© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 1

Table S1. Crystal data and structure refinement for $[\{CpRu(dippe)\}_2(\mu\text{-}N_2)][BAr'_4]_2\cdot FPh$ - **1a**.

Identification code	pvfj3fr
Empirical formula	C108 H103 B2 F49 N2 P4 Ru2
Formula weight	2707.56
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$ (no. 2)
Unit cell dimensions	a = 13.986(4) Å α = 83.25(1) deg. b = 14.321(4) Å β = 69.96(1) deg. c = 15.273(5) Å γ = 85.60(1) deg.
Volume	2851.8(15) $Å^3$
Z, Calculated density	1, 1.577 Mg/m^3
Absorption coefficient	0.449 mm^{-1}
F(000)	1364
Crystal size	0.80 x 0.60 x 0.32 mm, yellow block
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 10 sec. per frame full sphere data collection, 5 x 606 frames
Theta range for data collection	1.92 to 30.00 deg.
Index ranges	-19 <= h <= 19, -19 <= k <= 20, -21 <= l <= 21
Reflections collected / unique	52172 / 16347 [R(int)=0.0166, R(sigma)=0.0137]
Completeness to theta = 30.00	98.2%
Absorption correction	semi-empirical from equivalents (prg. SADABS)
Max. and min. transmission	0.83 and 0.74
Structure solution	direct methods (program SHELXS97)
Refinement method	full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	16347 / 36 / 758
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0963 (14834 data)
R indices (all data)	R1 = 0.0409, wR2 = 0.1020 (16347 data)
Extinction coefficient	0.0025(3)
Largest diff. peak and hole	0.924 and -0.638 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[\{CpRu(dippe)\}_2(\mu\text{-}N_2)][BAr'_4]_2\cdot FPh$ - **1a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	34108(1)	57160(1)	47064(1)	23(1)
P(1)	41446(3)	62451(3)	31282(3)	26(1)
P(2)	33034(3)	43234(3)	40934(3)	25(1)
N	46790(10)	51613(9)	48868(9)	24(1)
C(1)	19455(15)	65178(15)	50913(15)	39(1)
C(2)	27018(16)	71245(14)	51005(15)	41(1)
C(3)	31142(17)	67359(15)	57864(15)	42(1)
C(4)	25994(16)	58955(15)	62316(13)	41(1)
C(5)	18747(14)	57678(15)	58073(14)	40(1)
C(6)	44325(15)	52473(13)	24004(12)	34(1)
C(7)	44063(14)	43090(13)	30073(13)	32(1)
C(11)	53589(14)	68508(13)	27837(13)	33(1)
C(12)	52253(17)	76951(15)	33499(17)	45(1)
C(13)	62385(14)	61833(14)	28583(14)	37(1)
C(14)	33452(16)	70917(15)	26311(14)	39(1)
C(15)	23687(17)	66573(18)	26489(17)	48(1)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 2

C(16)		39190(20)	75360(20)	16403(18)	62(1)
C(21)		34931(14)	32433(12)	48257(14)	33(1)
C(22)		25213(18)	29985(16)	56456(16)	46(1)
C(23)		39810(20)	23753(15)	43172(19)	50(1)
C(24)		22290(14)	41816(14)	36762(14)	35(1)
C(25)		11739(16)	44219(19)	43657(18)	49(1)
C(26)		22354(19)	32226(17)	33252(17)	48(1)
B		-2760(14)	81225(12)	79965(13)	27(1)
C(31)		-7495(13)	70684(12)	83125(11)	29(1)
C(32)		-1912(15)	62319(12)	80555(13)	35(1)
C(33)		-6373(17)	53565(13)	83140(15)	42(1)
C(34)		-16629(17)	52804(14)	88273(15)	43(1)
C(35)		-22320(15)	60991(14)	90664(13)	37(1)
C(36)		-17884(14)	69732(13)	88176(13)	33(1)
C(37)		-80(20)	44756(16)	80360(20)	68(1)
C(38)		-33522(18)	60521(19)	96013(18)	51(1)
C(41)		-6441(13)	85412(11)	71084(12)	27(1)
C(42)		-931(13)	83908(11)	61764(12)	28(1)
C(43)		-4583(13)	87120(12)	54465(12)	30(1)
C(44)		-13926(15)	91949(13)	56143(13)	33(1)
C(45)		-19560(14)	93423(12)	65337(13)	33(1)
C(46)		-15963(14)	90168(12)	72616(13)	31(1)
C(47)		1442(15)	85015(14)	44648(13)	36(1)
C(48)		-29766(17)	98507(17)	67556(17)	46(1)
C(51)		-7368(13)	87961(12)	88624(12)	28(1)
C(52)		-10578(15)	84423(13)	98040(13)	34(1)
C(53)		-14119(16)	90307(15)	105216(14)	40(1)
C(54)		-14554(16)	100021(15)	103266(15)	40(1)
C(55)		-11370(16)	103641(13)	93980(15)	37(1)
C(56)		-7714(15)	97785(12)	86806(13)	33(1)
C(57)		-17880(30)	86240(20)	115258(17)	69(1)
C(58)		-12450(20)	114047(16)	91770(19)	56(1)
C(61)		9607(13)	81145(12)	77618(11)	28(1)
C(62)		14364(14)	75034(13)	82906(12)	32(1)
C(63)		24629(15)	75472(14)	81728(13)	34(1)
C(64)		30626(15)	82184(15)	75351(13)	36(1)
C(65)		26132(14)	88372(13)	70062(13)	33(1)
C(66)		15877(14)	87853(12)	71145(12)	31(1)
C(67)		29381(17)	68206(17)	87047(15)	46(1)
C(68)		32731(17)	95308(16)	62837(16)	43(1)
F(37A)		9650(14)	45489(12)	78983(18)	86(1)
F(37B)		90(20)	42756(16)	71684(19)	106(1)
F(37C)		-3520(20)	37395(12)	86020(20)	135(1)
F(38A)		-36857(16)	52004(16)	97910(30)	128(1)
F(38B)		-39088(16)	64930(30)	91440(20)	134(1)
F(38C)		-36255(18)	64240(30)	103760(20)	150(2)
F(47A)		-783(13)	90968(12)	38192(9)	63(1)
F(47B)		-28(12)	76266(10)	43112(10)	55(1)
F(47C)		11518(10)	85307(10)	42684(9)	48(1)
F(48A)		-30845(18)	103860(20)	60240(15)	109(1)
F(48B)		-37304(13)	92738(15)	70680(20)	101(1)
F(48C)		-31408(14)	104282(13)	74068(14)	75(1)
F(57A)		-15790(30)	77210(15)	116526(13)	119(1)
F(57B)		-27590(20)	87300(40)	118900(20)	193(2)
F(57C)		-14470(30)	90310(20)	120668(14)	141(1)
F(58A)		-8760(30)	116812(12)	82796(15)	130(1)
F(58B)		-22201(19)	117033(14)	94660(20)	116(1)
F(58C)		-8140(14)	119004(10)	96114(13)	64(1)
F(67A)		37809(17)	70937(17)	87918(18)	98(1)
F(67B)		32336(17)	60472(13)	82562(13)	81(1)
F(67C)		23298(14)	65533(13)	95511(10)	70(1)
F(68A)		27541(12)	102488(11)	60013(12)	61(1)
F(68B)		38272(14)	91188(13)	55095(11)	70(1)
F(68C)		39432(15)	98988(15)	65698(14)	80(1)
C(71)	#	55210(50)	-7360(40)	-3070(50)	225(8)
C(72)		58230(50)	-2260(70)	1710(50)	253(10)
C(73)		53020(70)	5100(50)	4780(50)	247(9)
F(71)		59840(110)	-13880(90)	-5800(100)	760(40)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 3

Remarks: C(71) through F(71) are from a disordered fluorobenzene molecule arranged about a centre of inversion. C(71), C(72), and C(73) have occupancy 1.0, F(71) occupancy 0.5. The fluorobenzene molecule was idealized by using SADI and FLAT restraints.

Table S3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [{CpRu(dippe)}$_2$(î-N $_2$)][BAr'$_4$]$_2$·FPh - **1a**.

	x	y	z	U_{eq}
H(1)	1563	6598	4686	47
H(2)	2892	7688	4714	49
H(3)	3640	6986	5928	50
H(4)	2722	5498	6720	49
H(5)	1423	5273	5969	48
H(6A)	3932	5253	2081	40
H(6B)	5108	5314	1922	40
H(7A)	5035	4210	3159	39
H(7B)	4359	3790	2661	39
H(11)	5527	7099	2118	40
H(12A)	5866	8008	3165	67
H(12B)	5018	7480	4012	67
H(12C)	4708	8132	3232	67
H(13A)	6858	6530	2672	55
H(13B)	6332	5688	2450	55
H(13C)	6085	5907	3500	55
H(14)	3131	7611	3040	47
H(15A)	1977	7122	2384	72
H(15B)	1966	6455	3290	72
H(15C)	2545	6120	2284	72
H(16A)	3462	7968	1422	93
H(16B)	4170	7045	1221	93
H(16C)	4488	7875	1652	93
H(21)	3981	3412	5117	39
H(22A)	2649	2432	6011	69
H(22B)	1983	2894	5407	69
H(22C)	2316	3514	6038	69
H(23A)	4040	1860	4771	75
H(23B)	4652	2521	3878	75
H(23C)	3559	2195	3981	75
H(24)	2327	4647	3123	42
H(25A)	658	4329	4095	74
H(25B)	1141	5073	4494	74
H(25C)	1054	4016	4945	74
H(26A)	1655	3199	3120	72
H(26B)	2197	2730	3828	72
H(26C)	2859	3132	2805	72
H(32)	505	6259	7698	42
H(34)	-1961	4691	9007	51
H(36)	-2200	7517	8994	39
H(42)	542	8064	6038	33
H(44)	-1635	9415	5122	40
H(46)	-2004	9118	7878	37
H(52)	-1034	7788	9958	41
H(54)	-1694	10400	10811	48
H(56)	-541	10048	8057	40
H(62)	1047	7049	8740	39
H(64)	3754	8254	7463	44
H(66)	1306	9212	6744	37
H(72)	6430	-393	296	304
H(73)	5524	885	830	297

All hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 4

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [{CpRu(dippe)}$_2$(î-N_2)][BAr'$_4$]$_2$·FPh - **1a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	20(1)	22(1)	24(1)	-3(1)	-6(1)	2(1)
P(1)	26(1)	26(1)	26(1)	0(1)	-8(1)	1(1)
P(2)	24(1)	25(1)	28(1)	-4(1)	-8(1)	-2(1)
N	23(1)	22(1)	24(1)	-3(1)	-5(1)	-2(1)
C(1)	30(1)	43(1)	41(1)	-11(1)	-10(1)	14(1)
C(2)	44(1)	28(1)	43(1)	-9(1)	-6(1)	11(1)
C(3)	42(1)	42(1)	42(1)	-22(1)	-13(1)	10(1)
C(4)	43(1)	44(1)	28(1)	-8(1)	-5(1)	16(1)
C(5)	28(1)	42(1)	39(1)	-8(1)	2(1)	4(1)
C(6)	36(1)	37(1)	26(1)	-6(1)	-7(1)	-1(1)
C(7)	31(1)	31(1)	32(1)	-10(1)	-6(1)	1(1)
C(11)	31(1)	31(1)	33(1)	5(1)	-7(1)	-4(1)
C(12)	42(1)	32(1)	58(1)	-3(1)	-12(1)	-8(1)
C(13)	28(1)	41(1)	38(1)	1(1)	-7(1)	-3(1)
C(14)	38(1)	40(1)	39(1)	7(1)	-16(1)	5(1)
C(15)	41(1)	57(1)	49(1)	6(1)	-23(1)	5(1)
C(16)	53(1)	77(2)	48(1)	27(1)	-18(1)	3(1)
C(21)	36(1)	25(1)	40(1)	-2(1)	-16(1)	-3(1)
C(22)	47(1)	44(1)	44(1)	9(1)	-15(1)	-12(1)
C(23)	64(1)	28(1)	63(1)	-10(1)	-26(1)	5(1)
C(24)	33(1)	39(1)	39(1)	0(1)	-17(1)	-8(1)
C(25)	30(1)	60(1)	61(1)	-5(1)	-18(1)	-7(1)
C(26)	54(1)	50(1)	50(1)	-8(1)	-25(1)	-17(1)
B	29(1)	22(1)	27(1)	-3(1)	-8(1)	2(1)
C(31)	34(1)	25(1)	25(1)	-3(1)	-8(1)	0(1)
C(32)	37(1)	26(1)	34(1)	-2(1)	-2(1)	-2(1)
C(33)	46(1)	25(1)	44(1)	-1(1)	-1(1)	-1(1)
C(34)	49(1)	31(1)	38(1)	2(1)	-3(1)	-10(1)
C(35)	36(1)	38(1)	31(1)	-2(1)	-5(1)	-7(1)
C(36)	33(1)	32(1)	32(1)	-6(1)	-8(1)	0(1)
C(37)	61(2)	27(1)	88(2)	-4(1)	10(1)	-3(1)
C(38)	39(1)	55(1)	52(1)	-4(1)	-3(1)	-12(1)
C(41)	30(1)	22(1)	28(1)	-3(1)	-9(1)	1(1)
C(42)	29(1)	25(1)	29(1)	-3(1)	-10(1)	2(1)
C(43)	33(1)	27(1)	27(1)	-2(1)	-9(1)	1(1)
C(44)	39(1)	30(1)	35(1)	-4(1)	-17(1)	4(1)
C(45)	32(1)	29(1)	39(1)	-7(1)	-15(1)	6(1)
C(46)	32(1)	29(1)	32(1)	-6(1)	-10(1)	3(1)
C(47)	41(1)	36(1)	29(1)	-2(1)	-12(1)	1(1)
C(48)	42(1)	48(1)	52(1)	-15(1)	-20(1)	15(1)
C(51)	28(1)	27(1)	29(1)	-5(1)	-9(1)	1(1)
C(52)	37(1)	30(1)	32(1)	-4(1)	-6(1)	-5(1)
C(53)	42(1)	42(1)	30(1)	-8(1)	-3(1)	-7(1)
C(54)	42(1)	39(1)	39(1)	-17(1)	-12(1)	5(1)
C(55)	45(1)	28(1)	44(1)	-11(1)	-24(1)	8(1)
C(56)	43(1)	27(1)	33(1)	-4(1)	-18(1)	2(1)
C(57)	93(2)	62(2)	33(1)	-10(1)	10(1)	-23(2)
C(58)	92(2)	32(1)	65(2)	-17(1)	-53(2)	20(1)
C(61)	30(1)	27(1)	26(1)	-5(1)	-9(1)	2(1)
C(62)	34(1)	32(1)	29(1)	-3(1)	-9(1)	4(1)
C(63)	36(1)	38(1)	29(1)	-7(1)	-12(1)	9(1)
C(64)	31(1)	45(1)	34(1)	-11(1)	-12(1)	4(1)
C(65)	33(1)	34(1)	31(1)	-6(1)	-9(1)	-3(1)
C(66)	34(1)	28(1)	32(1)	-3(1)	-12(1)	-1(1)
C(67)	43(1)	53(1)	39(1)	-4(1)	-16(1)	15(1)
C(68)	40(1)	45(1)	44(1)	-1(1)	-11(1)	-9(1)
F(37A)	63(1)	42(1)	132(2)	-1(1)	-12(1)	15(1)
F(37B)	115(2)	76(1)	113(2)	-57(1)	-8(1)	12(1)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 5

F(37C)	116(2)	30(1)	168(2)	27(1)	52(2)	13(1)
F(38A)	53(1)	73(1)	215(3)	-5(2)	13(2)	-27(1)
F(38B)	43(1)	196(3)	132(2)	57(2)	-15(1)	1(1)
F(38C)	67(1)	258(4)	104(2)	-105(2)	38(1)	-60(2)
F(47A)	74(1)	77(1)	31(1)	4(1)	-16(1)	25(1)
F(47B)	63(1)	51(1)	49(1)	-23(1)	-7(1)	-10(1)
F(47C)	40(1)	57(1)	40(1)	-3(1)	-3(1)	-3(1)
F(48A)	91(1)	156(2)	69(1)	-4(1)	-33(1)	81(2)
F(48B)	35(1)	83(1)	181(2)	-48(2)	-23(1)	6(1)
F(48C)	70(1)	72(1)	93(1)	-46(1)	-36(1)	39(1)
F(57A)	221(3)	63(1)	39(1)	8(1)	-3(1)	-24(2)
F(57B)	98(2)	297(5)	97(2)	62(3)	52(2)	6(3)
F(57C)	273(4)	113(2)	39(1)	5(1)	-44(2)	-81(2)
F(58A)	298(4)	35(1)	69(1)	-6(1)	-81(2)	30(1)
F(58B)	105(2)	59(1)	228(3)	-46(2)	-113(2)	43(1)
F(58C)	93(1)	33(1)	85(1)	-13(1)	-53(1)	3(1)
F(67A)	82(1)	105(2)	130(2)	35(1)	-79(1)	-14(1)
F(67B)	107(2)	69(1)	67(1)	-23(1)	-37(1)	54(1)
F(67C)	73(1)	76(1)	41(1)	13(1)	-8(1)	34(1)
F(68A)	56(1)	48(1)	68(1)	17(1)	-12(1)	-9(1)
F(68B)	69(1)	69(1)	48(1)	-2(1)	11(1)	-5(1)
F(68C)	77(1)	91(1)	83(1)	17(1)	-40(1)	-50(1)
C(71)	169(9)	162(8)	207(11)	75(8)	67(8)	70(8)
C(72)	134(7)	470(30)	167(10)	107(13)	-86(8)	-117(12)
C(73)	313(19)	230(13)	135(7)	-46(8)	45(9)	-154(13)
F(71)	510(30)	160(12)	1070(80)	100(20)	350(40)	163(18)

Table S5. Bond lengths [Å] and angles [deg] for [{CpRu(dippe)}$_2$(i-N $_2$)][BAr'$_4$]$_2$·FPh - **1a**.

Bond distances

Ru-N	1.9800(14)
Ru-C(1)	2.1991(18)
Ru-C(5)	2.2310(19)
Ru-C(2)	2.2325(19)
Ru-C(3)	2.2430(19)
Ru-C(4)	2.250(2)
Ru-P(1)	2.3306(8)
Ru-P(2)	2.3361(7)
P(1)-C(6)	1.8488(19)
P(1)-C(11)	1.8492(19)
P(1)-C(14)	1.8585(19)
P(2)-C(7)	1.8388(18)
P(2)-C(24)	1.8543(19)
P(2)-C(21)	1.8568(19)
N-N#1	1.118(3)
C(1)-C(5)	1.423(3)
C(1)-C(2)	1.424(3)
C(1)-H(1)	0.94
C(2)-C(3)	1.403(3)
C(2)-H(2)	0.94
C(3)-C(4)	1.426(3)
C(3)-H(3)	0.94
C(4)-C(5)	1.410(3)
C(4)-H(4)	0.94
C(5)-H(5)	0.94
C(6)-C(7)	1.535(3)
C(6)-H(6A)	0.98
C(6)-H(6B)	0.98
C(7)-H(7A)	0.98
C(7)-H(7B)	0.98
C(11)-C(13)	1.527(3)
C(11)-C(12)	1.531(3)
C(11)-H(11)	0.99
C(12)-H(12A)	0.97
C(12)-H(12B)	0.97
C(12)-H(12C)	0.97
C(13)-H(13A)	0.97
C(13)-H(13B)	0.97
C(13)-H(13C)	0.97
C(14)-C(15)	1.534(3)
C(14)-C(16)	1.536(3)
C(14)-H(14)	0.99
C(15)-H(15A)	0.97
C(15)-H(15B)	0.97
C(15)-H(15C)	0.97
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
C(16)-H(16C)	0.97
C(21)-C(22)	1.530(3)
C(21)-C(23)	1.532(3)
C(21)-H(21)	0.99
C(22)-H(22A)	0.97
C(22)-H(22B)	0.97
C(22)-H(22C)	0.97
C(23)-H(23A)	0.97
C(23)-H(23B)	0.97
C(23)-H(23C)	0.97
C(24)-C(26)	1.530(3)
C(24)-C(25)	1.532(3)
C(24)-H(24)	0.99
C(25)-H(25A)	0.97
C(25)-H(25B)	0.97
C(25)-H(25C)	0.97

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 6

C(26)-H(26A)	0.97
C(26)-H(26B)	0.97
C(26)-H(26C)	0.97
B-C(61)	1.641(3)
B-C(41)	1.645(3)
B-C(31)	1.647(3)
B-C(51)	1.648(2)
C(31)-C(32)	1.399(2)
C(31)-C(36)	1.401(2)
C(32)-C(33)	1.397(3)
C(32)-H(32)	0.94
C(33)-C(34)	1.385(3)
C(33)-C(37)	1.499(3)
C(34)-C(35)	1.378(3)
C(34)-H(34)	0.94
C(35)-C(36)	1.394(3)
C(35)-C(38)	1.501(3)
C(36)-H(36)	0.94
C(37)-F(37C)	1.291(3)
C(37)-F(37A)	1.314(4)
C(37)-F(37B)	1.381(4)
C(38)-F(38C)	1.280(3)
C(38)-F(38B)	1.298(4)
C(38)-F(38A)	1.304(3)
C(41)-C(42)	1.400(2)
C(41)-C(46)	1.406(2)
C(42)-C(43)	1.396(2)
C(42)-H(42)	0.94
C(43)-C(44)	1.387(3)
C(43)-C(47)	1.500(3)
C(44)-C(45)	1.387(3)
C(44)-H(44)	0.94
C(45)-C(46)	1.390(3)
C(45)-C(48)	1.500(3)
C(46)-H(46)	0.94
C(47)-F(47A)	1.330(2)
C(47)-F(47C)	1.339(2)
C(47)-F(47B)	1.345(2)
C(48)-F(48B)	1.311(3)
C(48)-F(48C)	1.317(3)
C(48)-F(48A)	1.325(3)
C(51)-C(52)	1.396(2)
C(51)-C(56)	1.402(2)
C(52)-C(53)	1.392(3)
C(52)-H(52)	0.94
C(53)-C(54)	1.389(3)
C(53)-C(57)	1.501(3)
C(54)-C(55)	1.381(3)
C(54)-H(54)	0.94
C(55)-C(56)	1.390(3)
C(55)-C(58)	1.497(3)
C(56)-H(56)	0.94
C(57)-F(57B)	1.284(5)
C(57)-F(57C)	1.294(4)
C(57)-F(57A)	1.311(4)
C(58)-F(58A)	1.312(4)
C(58)-F(58C)	1.326(3)
C(58)-F(58B)	1.334(4)
C(61)-C(62)	1.405(2)
C(61)-C(66)	1.408(2)
C(62)-C(63)	1.390(3)
C(62)-H(62)	0.94
C(63)-C(64)	1.386(3)
C(63)-C(67)	1.500(3)
C(64)-C(65)	1.388(3)
C(64)-H(64)	0.94
C(65)-C(66)	1.393(3)
C(65)-C(68)	1.497(3)
C(66)-H(66)	0.94
C(67)-F(67C)	1.312(3)
C(67)-F(67A)	1.323(3)
C(67)-F(67B)	1.334(3)
C(68)-F(68C)	1.326(3)
C(68)-F(68A)	1.329(3)
C(68)-F(68B)	1.346(3)
C(71)-F(71)	1.131(13)
C(71)-C(73)#2	1.275(5)
C(71)-C(72)	1.275(5)
C(72)-C(73)	1.275(5)
C(72)-H(72)	0.94
C(73)-C(71)#2	1.275(5)
C(73)-H(73)	0.94

Bond angles

N-Ru-C(1)	155.37(7)
N-Ru-C(5)	126.07(7)
C(1)-Ru-C(5)	37.47(8)
N-Ru-C(2)	125.69(7)
C(1)-Ru-C(2)	37.48(8)
C(5)-Ru-C(2)	61.93(8)
N-Ru-C(3)	94.66(7)
C(1)-Ru-C(3)	62.05(8)
C(5)-Ru-C(3)	61.61(8)
C(2)-Ru-C(3)	36.53(8)
N-Ru-C(4)	94.78(7)
C(1)-Ru-C(4)	62.08(8)
C(5)-Ru-C(4)	36.67(8)
C(2)-Ru-C(4)	61.52(8)
C(3)-Ru-C(4)	37.01(8)
N-Ru-P(1)	96.51(4)
C(1)-Ru-P(1)	101.85(6)
C(5)-Ru-P(1)	137.38(6)
C(2)-Ru-P(1)	93.59(6)
C(3)-Ru-P(1)	119.17(7)
C(4)-Ru-P(1)	154.63(6)
N-Ru-P(2)	87.06(4)
C(1)-Ru-P(2)	111.34(6)
C(5)-Ru-P(2)	99.62(6)
C(2)-Ru-P(2)	147.22(6)
C(3)-Ru-P(2)	157.69(6)
C(4)-Ru-P(2)	120.68(6)
P(1)-Ru-P(2)	82.60(2)
C(6)-P(1)-C(11)	104.82(9)
C(6)-P(1)-C(14)	104.98(10)
C(11)-P(1)-C(14)	102.72(9)
C(6)-P(1)-Ru	110.41(6)
C(11)-P(1)-Ru	116.98(6)
C(14)-P(1)-Ru	115.68(7)
C(7)-P(2)-C(24)	102.19(9)
C(7)-P(2)-C(21)	104.56(9)
C(24)-P(2)-C(21)	109.83(9)
C(7)-P(2)-Ru	104.95(6)
C(24)-P(2)-Ru	119.69(7)
C(21)-P(2)-Ru	113.66(6)
N#1-N-Ru	170.65(17)
C(5)-C(1)-C(2)	107.53(18)
C(5)-C(1)-Ru	72.48(10)

C(2)-C(1)-Ru	72.53(11)
C(5)-C(1)-H(1)	126.2
C(2)-C(1)-H(1)	126.2
Ru-C(1)-H(1)	120.6
C(3)-C(2)-C(1)	108.18(19)
C(3)-C(2)-Ru	72.14(11)
C(1)-C(2)-Ru	69.99(11)
C(3)-C(2)-H(2)	125.9
C(1)-C(2)-H(2)	125.9
Ru-C(2)-H(2)	123.6
C(2)-C(3)-C(4)	108.28(19)
C(2)-C(3)-Ru	71.32(11)
C(4)-C(3)-Ru	71.78(11)
C(2)-C(3)-H(3)	125.9
C(4)-C(3)-H(3)	125.9
Ru-C(3)-H(3)	122.7
C(5)-C(4)-C(3)	107.77(18)
C(5)-C(4)-Ru	70.92(11)
C(3)-C(4)-Ru	71.21(11)
C(5)-C(4)-H(4)	126.1
C(3)-C(4)-H(4)	126.1
Ru-C(4)-H(4)	123.4
C(4)-C(5)-C(1)	108.20(19)
C(4)-C(5)-Ru	72.42(11)
C(1)-C(5)-Ru	70.05(11)
C(4)-C(5)-H(5)	125.9
C(1)-C(5)-H(5)	125.9
Ru-C(5)-H(5)	123.3
C(7)-C(6)-P(1)	110.61(12)
C(7)-C(6)-H(6A)	109.5
P(1)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6B)	109.5
P(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1
C(6)-C(7)-P(2)	109.76(12)
C(6)-C(7)-H(7A)	109.7
P(2)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7B)	109.7
P(2)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(13)-C(11)-C(12)	112.19(17)
C(13)-C(11)-P(1)	112.33(13)
C(12)-C(11)-P(1)	110.07(13)
C(13)-C(11)-H(11)	107.3
C(12)-C(11)-H(11)	107.3
P(1)-C(11)-H(11)	107.3
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(16)	110.11(19)
C(15)-C(14)-P(1)	112.32(15)
C(16)-C(14)-P(1)	113.57(15)
C(15)-C(14)-H(14)	106.8
C(16)-C(14)-H(14)	106.8
P(1)-C(14)-H(14)	106.8
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(22)-C(21)-C(23)	111.24(18)
C(22)-C(21)-P(2)	111.81(14)
C(23)-C(21)-P(2)	117.13(15)
C(22)-C(21)-H(21)	105.2
C(23)-C(21)-H(21)	105.2
P(2)-C(21)-H(21)	105.2
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(26)-C(24)-C(25)	110.26(17)
C(26)-C(24)-P(2)	114.02(15)
C(25)-C(24)-P(2)	114.74(15)
C(26)-C(24)-H(24)	105.6
C(25)-C(24)-H(24)	105.6
P(2)-C(24)-H(24)	105.6
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(61)-B-C(41)	113.94(14)
C(61)-B-C(31)	113.33(13)
C(41)-B-C(31)	104.81(13)
C(61)-B-C(51)	103.92(13)
C(41)-B-C(51)	110.42(13)
C(31)-B-C(51)	110.54(13)
C(32)-C(31)-C(36)	115.68(16)
C(32)-C(31)-B	124.12(15)
C(36)-C(31)-B	120.05(15)
C(33)-C(32)-C(31)	121.95(18)
C(33)-C(32)-H(32)	119.0
C(31)-C(32)-H(32)	119.0
C(34)-C(33)-C(32)	121.20(18)
C(34)-C(33)-C(37)	118.56(19)
C(32)-C(33)-C(37)	120.2(2)
C(35)-C(34)-C(33)	117.72(18)
C(35)-C(34)-H(34)	121.1
C(33)-C(34)-H(34)	121.1
C(34)-C(35)-C(36)	121.28(18)
C(34)-C(35)-C(38)	119.55(19)
C(36)-C(35)-C(38)	119.17(19)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 8

C(35)-C(36)-C(31)	122.14(17)
C(35)-C(36)-H(36)	118.9
C(31)-C(36)-H(36)	118.9
F(37C)-C(37)-F(37A)	110.2(3)
F(37C)-C(37)-F(37B)	105.8(3)
F(37A)-C(37)-F(37B)	102.0(2)
F(37C)-C(37)-C(33)	113.5(2)
F(37A)-C(37)-C(33)	113.8(2)
F(37B)-C(37)-C(33)	110.7(3)
F(38C)-C(38)-F(38B)	104.8(3)
F(38C)-C(38)-F(38A)	107.1(3)
F(38B)-C(38)-F(38A)	103.8(3)
F(38C)-C(38)-C(35)	113.5(2)
F(38B)-C(38)-C(35)	112.9(2)
F(38A)-C(38)-C(35)	113.9(2)
C(42)-C(41)-C(46)	115.65(15)
C(42)-C(41)-B	123.64(14)
C(46)-C(41)-B	120.51(15)
C(43)-C(42)-C(41)	121.99(16)
C(43)-C(42)-H(42)	119.0
C(41)-C(42)-H(42)	119.0
C(44)-C(43)-C(42)	121.23(16)
C(44)-C(43)-C(47)	118.85(16)
C(42)-C(43)-C(47)	119.87(16)
C(45)-C(44)-C(43)	117.72(16)
C(45)-C(44)-H(44)	121.1
C(43)-C(44)-H(44)	121.1
C(44)-C(45)-C(46)	121.09(17)
C(44)-C(45)-C(48)	119.91(17)
C(46)-C(45)-C(48)	118.99(18)
C(45)-C(46)-C(41)	122.30(16)
C(45)-C(46)-H(46)	118.9
C(41)-C(46)-H(46)	118.9
F(47A)-C(47)-F(47C)	106.14(17)
F(47A)-C(47)-F(47B)	107.58(17)
F(47C)-C(47)-F(47B)	104.69(16)
F(47A)-C(47)-C(43)	113.07(16)
F(47C)-C(47)-C(43)	113.07(16)
F(47B)-C(47)-C(43)	111.73(16)
F(48B)-C(48)-F(48C)	105.7(2)
F(48B)-C(48)-F(48A)	107.7(2)
F(48C)-C(48)-F(48A)	104.9(2)
F(48B)-C(48)-C(45)	112.4(2)
F(48C)-C(48)-C(45)	112.90(18)
F(48A)-C(48)-C(45)	112.7(2)
C(52)-C(51)-C(56)	116.20(16)
C(52)-C(51)-B	123.15(15)
C(56)-C(51)-B	120.56(15)
C(53)-C(52)-C(51)	121.89(18)
C(53)-C(52)-H(52)	119.1
C(51)-C(52)-H(52)	119.1
C(54)-C(53)-C(52)	121.02(18)
C(54)-C(53)-C(57)	118.51(19)
C(52)-C(53)-C(57)	120.4(2)
C(55)-C(54)-C(53)	117.82(17)
C(55)-C(54)-H(54)	121.1
C(53)-C(54)-H(54)	121.1
C(54)-C(55)-C(56)	121.25(18)
C(54)-C(55)-C(58)	118.35(19)
C(56)-C(55)-C(58)	120.32(19)
C(55)-C(56)-C(51)	121.79(17)
C(55)-C(56)-H(56)	119.1
C(51)-C(56)-H(56)	119.1
F(57B)-C(57)-F(57C)	103.7(3)
F(57B)-C(57)-F(57A)	105.9(3)
F(57C)-C(57)-F(57A)	106.7(3)
F(57B)-C(57)-C(53)	111.6(3)
F(57C)-C(57)-C(53)	113.8(2)
F(57A)-C(57)-C(53)	114.3(2)
F(58A)-C(58)-F(58C)	107.4(3)
F(58A)-C(58)-F(58B)	106.4(3)
F(58C)-C(58)-F(58B)	104.0(2)
F(58A)-C(58)-C(55)	113.6(2)
F(58C)-C(58)-C(55)	113.36(18)
F(58B)-C(58)-C(55)	111.4(3)
C(62)-C(61)-C(66)	115.63(16)
C(62)-C(61)-B	121.00(15)
C(66)-C(61)-B	122.88(15)
C(63)-C(62)-C(61)	122.27(17)
C(63)-C(62)-H(62)	118.9
C(61)-C(62)-H(62)	118.9
C(64)-C(63)-C(62)	120.98(17)
C(64)-C(63)-C(67)	119.69(18)
C(62)-C(63)-C(67)	119.23(19)
C(63)-C(64)-C(65)	118.14(18)
C(63)-C(64)-H(64)	120.9
C(65)-C(64)-H(64)	120.9
C(64)-C(65)-C(66)	120.91(18)
C(64)-C(65)-C(68)	118.12(18)
C(66)-C(65)-C(68)	120.90(18)
C(65)-C(66)-C(61)	122.05(17)
C(65)-C(66)-H(66)	119.0
C(61)-C(66)-H(66)	119.0
F(67C)-C(67)-F(67A)	106.9(2)
F(67C)-C(67)-F(67B)	106.9(2)
F(67A)-C(67)-F(67B)	104.2(2)
F(67C)-C(67)-C(63)	113.81(18)
F(67A)-C(67)-C(63)	113.5(2)
F(67B)-C(67)-C(63)	111.04(18)
F(68C)-C(68)-F(68A)	106.6(2)
F(68C)-C(68)-F(68B)	105.6(2)
F(68A)-C(68)-F(68B)	106.2(2)
F(68C)-C(68)-C(65)	113.18(19)
F(68A)-C(68)-C(65)	113.69(18)
F(68B)-C(68)-C(65)	111.01(18)
F(71)-C(71)-C(73)#2	119.99(7)
F(71)-C(71)-C(72)	119.98(7)
C(73)#2-C(71)-C(72)	120.04(8)
C(73)-C(72)-C(71)	119.98(8)
C(73)-C(72)-H(72)	120.0
C(71)-C(72)-H(72)	120.0
C(71)#2-C(73)-C(72)	119.98(8)
C(71)#2-C(73)-H(73)	120.0
C(72)-C(73)-H(73)	120.0

Torsion angles

N-Ru-P1-C6	74.89(8)
C1-Ru-P1-C6	-121.62(9)
C5-Ru-P1-C6	-107.46(11)
C2-Ru-P1-C6	-158.56(9)
C3-Ru-P1-C6	173.94(9)
C4-Ru-P1-C6	-169.23(15)
P2-Ru-P1-C6	-11.28(7)
N-Ru-P1-C11	-44.83(8)
C1-Ru-P1-C11	118.66(9)
C5-Ru-P1-C11	132.82(11)
C2-Ru-P1-C11	81.72(9)
C3-Ru-P1-C11	54.22(9)
C4-Ru-P1-C11	71.05(16)
P2-Ru-P1-C11	-131.00(7)
N-Ru-P1-C14	-166.10(9)
C1-Ru-P1-C14	-2.61(10)
C5-Ru-P1-C14	11.55(12)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 9

C2-Ru-P1-C14	-39.55(10)
C3-Ru-P1-C14	-67.05(10)
C4-Ru-P1-C14	-50.22(16)
P2-Ru-P1-C14	107.74(8)
N-Ru-P2-C7	-65.76(8)
C1-Ru-P2-C7	131.08(9)
C5-Ru-P2-C7	168.13(9)
C2-Ru-P2-C7	116.32(12)
C3-Ru-P2-C7	-160.87(16)
C4-Ru-P2-C7	-159.58(9)
P1-Ru-P2-C7	31.20(7)
N-Ru-P2-C24	-179.58(8)
C1-Ru-P2-C24	17.26(10)
C5-Ru-P2-C24	54.31(9)
C2-Ru-P2-C24	2.50(13)
C3-Ru-P2-C24	85.31(17)
C4-Ru-P2-C24	86.60(10)
P1-Ru-P2-C24	-82.62(8)
N-Ru-P2-C21	47.88(8)
C1-Ru-P2-C21	-115.28(9)
C5-Ru-P2-C21	-78.22(9)
C2-Ru-P2-C21	-130.04(12)
C3-Ru-P2-C21	-47.22(17)
C4-Ru-P2-C21	-45.93(9)
P1-Ru-P2-C21	144.84(7)
C1-Ru-N-N#1	30.7(11)
C5-Ru-N-N#1	-9.2(11)
C2-Ru-N-N#1	69.7(10)
C3-Ru-N-N#1	48.8(10)
C4-Ru-N-N#1	11.6(10)
P1-Ru-N-N#1	168.9(10)
P2-Ru-N-N#1	-108.9(10)
N-Ru-C1-C5	-58.4(2)
C2-Ru-C1-C5	-115.50(18)
C3-Ru-C1-C5	-78.90(14)
C4-Ru-C1-C5	-36.79(13)
P1-Ru-C1-C5	164.20(11)
P2-Ru-C1-C5	77.60(13)
N-Ru-C1-C2	57.1(2)
C5-Ru-C1-C2	115.50(18)
C3-Ru-C1-C2	36.60(13)
C4-Ru-C1-C2	78.71(14)
P1-Ru-C1-C2	-80.30(12)
P2-Ru-C1-C2	-166.90(11)
C5-C1-C2-C3	2.1(2)
Ru-C1-C2-C3	-62.41(13)
C5-C1-C2-Ru	64.51(13)
N-Ru-C2-C3	-36.70(16)
C1-Ru-C2-C3	117.79(18)
C5-Ru-C2-C3	79.31(14)
C4-Ru-C2-C3	37.46(13)
P1-Ru-C2-C3	-137.36(13)
P2-Ru-C2-C3	140.74(12)
N-Ru-C2-C1	-154.49(11)
C5-Ru-C2-C1	-38.48(12)
C3-Ru-C2-C1	-117.79(18)
C4-Ru-C2-C1	-80.33(14)
P1-Ru-C2-C1	104.85(12)
P2-Ru-C2-C1	22.96(18)
C1-C2-C3-C4	-1.6(2)
Ru-C2-C3-C4	-62.66(13)
C1-C2-C3-Ru	61.04(13)
N-Ru-C3-C2	150.86(13)
C1-Ru-C3-C2	-37.55(13)
C5-Ru-C3-C2	-80.28(14)
C4-Ru-C3-C2	-117.37(19)
P1-Ru-C3-C2	50.73(14)
P2-Ru-C3-C2	-115.54(17)
N-Ru-C3-C4	-91.77(12)
C1-Ru-C3-C4	79.83(14)
C5-Ru-C3-C4	37.10(12)
C2-Ru-C3-C4	117.37(19)
P1-Ru-C3-C4	168.11(10)
P2-Ru-C3-C4	1.8(2)
C2-C3-C4-C5	0.5(2)
Ru-C3-C4-C5	-61.85(13)
C2-C3-C4-Ru	62.37(13)
N-Ru-C4-C5	-151.29(12)
C1-Ru-C4-C5	37.59(12)
C2-Ru-C4-C5	80.34(13)
C3-Ru-C4-C5	117.32(18)
P1-Ru-C4-C5	92.48(18)
P2-Ru-C4-C5	-61.87(13)
N-Ru-C4-C3	91.40(12)
C1-Ru-C4-C3	-79.73(13)
C5-Ru-C4-C3	-117.32(18)
C2-Ru-C4-C3	-36.97(13)
P1-Ru-C4-C3	-24.8(2)
P2-Ru-C4-C3	-179.19(10)
C3-C4-C5-C1	0.8(2)
Ru-C4-C5-C1	-61.25(13)
C3-C4-C5-Ru	62.04(13)
C2-C1-C5-C4	-1.8(2)
Ru-C1-C5-C4	62.77(13)
C2-C1-C5-Ru	-64.55(13)
N-Ru-C5-C4	36.32(15)
C1-Ru-C5-C4	-117.61(18)
C2-Ru-C5-C4	-79.12(14)
C3-Ru-C5-C4	-37.44(12)
P1-Ru-C5-C4	-140.79(11)
P2-Ru-C5-C4	129.71(11)
N-Ru-C5-C1	153.94(11)
C2-Ru-C5-C1	38.49(13)
C3-Ru-C5-C1	80.17(14)
C4-Ru-C5-C1	117.61(18)
P1-Ru-C5-C1	-23.18(16)
P2-Ru-C5-C1	-112.67(12)
C11-P1-C6-C7	110.83(13)
C14-P1-C6-C7	-141.31(13)
Ru-P1-C6-C7	-15.98(14)
P1-C6-C7-P2	42.88(16)
C24-P2-C7-C6	74.47(14)
C21-P2-C7-C6	-171.03(12)
Ru-P2-C7-C6	-51.14(13)
C6-P1-C11-C13	-53.60(16)
C14-P1-C11-C13	-163.11(14)
Ru-P1-C11-C13	69.05(15)
C6-P1-C11-C12	-179.39(14)
C14-P1-C11-C12	71.10(16)
Ru-P1-C11-C12	-56.74(15)
C6-P1-C14-C15	58.66(18)
C11-P1-C14-C15	168.04(16)
Ru-P1-C14-C15	-63.30(18)
C6-P1-C14-C16	-67.1(2)
C11-P1-C14-C16	42.3(2)
Ru-P1-C14-C16	170.93(17)
C7-P2-C21-C22	-165.08(14)
C24-P2-C21-C22	-56.08(16)
Ru-P2-C21-C22	81.05(14)
C7-P2-C21-C23	-35.03(18)
C24-P2-C21-C23	73.97(18)
Ru-P2-C21-C23	-148.91(14)
C7-P2-C24-C26	66.76(16)
C21-P2-C24-C26	-43.81(18)
Ru-P2-C24-C26	-177.96(13)
C7-P2-C24-C25	-164.72(16)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 10

C21-P2-C24-C25	84.72(17)
Ru-P2-C24-C25	-49.44(17)
C61-B-C31-C32	-25.3(2)
C41-B-C31-C32	99.55(19)
C51-B-C31-C32	-141.47(17)
C61-B-C31-C36	159.24(15)
C41-B-C31-C36	-75.94(19)
C51-B-C31-C36	43.0(2)
C36-C31-C32-C33	-2.0(3)
B-C31-C32-C33	-177.68(19)
C31-C32-C33-C34	1.0(3)
C31-C32-C33-C37	-179.1(2)
C32-C33-C34-C35	0.7(3)
C37-C33-C34-C35	-179.2(2)
C33-C34-C35-C36	-1.3(3)
C33-C34-C35-C38	178.4(2)
C34-C35-C36-C31	0.2(3)
C38-C35-C36-C31	-179.50(19)
C32-C31-C36-C35	1.4(3)
B-C31-C36-C35	177.26(17)
C34-C33-C37-F37C	-27.3(5)
C32-C33-C37-F37C	152.8(3)
C34-C33-C37-F37A	-154.4(3)
C32-C33-C37-F37A	25.7(4)
C34-C33-C37-F37B	91.4(3)
C32-C33-C37-F37B	-88.5(3)
C34-C35-C38-F38C	122.8(3)
C36-C35-C38-F38C	-57.5(4)
C34-C35-C38-F38B	-118.2(3)
C36-C35-C38-F38B	61.6(3)
C34-C35-C38-F38A	-0.2(4)
C36-C35-C38-F38A	179.6(3)
C61-B-C41-C42	36.5(2)
C31-B-C41-C42	-87.93(18)
C51-B-C41-C42	153.01(15)
C61-B-C41-C46	-148.85(15)
C31-B-C41-C46	86.71(18)
C51-B-C41-C46	-32.3(2)
C46-C41-C42-C43	1.4(2)
B-C41-C42-C43	176.26(15)
C41-C42-C43-C44	-0.3(3)
C41-C42-C43-C47	-177.76(16)
C42-C43-C44-C45	-0.5(3)
C47-C43-C44-C45	177.06(17)
C43-C44-C45-C46	0.0(3)
C43-C44-C45-C48	-179.30(18)
C44-C45-C46-C41	1.2(3)
C48-C45-C46-C41	-179.48(18)
C42-C41-C46-C45	-1.9(3)
B-C41-C46-C45	-176.92(16)
C44-C43-C47-F47A	24.7(3)
C42-C43-C47-F47A	-157.70(18)
C44-C43-C47-F47C	145.39(17)
C42-C43-C47-F47C	-37.1(2)
C44-C43-C47-F47B	-96.8(2)
C42-C43-C47-F47B	80.8(2)
C44-C45-C48-F48B	100.0(3)
C46-C45-C48-F48B	-79.3(3)
C44-C45-C48-F48C	-140.6(2)
C46-C45-C48-F48C	40.1(3)
C44-C45-C48-F48A	-22.0(3)
C46-C45-C48-F48A	158.7(2)
C61-B-C51-C52	-93.85(19)
C41-B-C51-C52	143.58(17)
C31-B-C51-C52	28.1(2)
C61-B-C51-C56	82.52(19)
C41-B-C51-C56	-40.1(2)
C31-B-C51-C56	-155.58(16)
C56-C51-C52-C53	1.3(3)
B-C51-C52-C53	177.79(18)
C51-C52-C53-C54	-0.3(3)
C51-C52-C53-C57	177.7(2)
C52-C53-C54-C55	0.1(3)
C57-C53-C54-C55	-178.0(2)
C53-C54-C55-C56	-0.9(3)
C53-C54-C55-C58	175.9(2)
C54-C55-C56-C51	1.9(3)
C58-C55-C56-C51	-174.8(2)
C52-C51-C56-C55	-2.1(3)
B-C51-C56-C55	-178.69(17)
C54-C53-C57-F57B	69.6(4)
C52-C53-C57-F57B	-108.5(4)
C54-C53-C57-F57C	-47.4(4)
C52-C53-C57-F57C	134.5(3)
C54-C53-C57-F57A	-170.3(3)
C52-C53-C57-F57A	11.7(4)
C54-C55-C58-F58A	176.9(3)
C56-C55-C58-F58A	-6.3(4)
C54-C55-C58-F58C	54.0(3)
C56-C55-C58-F58C	-129.2(2)
C54-C55-C58-F58B	-63.0(3)
C56-C55-C58-F58B	113.8(3)
C41-B-C61-C62	-157.32(15)
C31-B-C61-C62	-37.6(2)
C51-B-C61-C62	82.45(18)
C41-B-C61-C66	31.1(2)
C31-B-C61-C66	150.80(16)
C51-B-C61-C66	-89.16(18)
C66-C61-C62-C63	-1.0(3)
B-C61-C62-C63	-173.19(16)
C61-C62-C63-C64	1.5(3)
C61-C62-C63-C67	-174.91(17)
C62-C63-C64-C65	-1.0(3)
C67-C63-C64-C65	175.40(18)
C63-C64-C65-C66	0.1(3)
C63-C64-C65-C68	-176.99(18)
C64-C65-C66-C61	0.4(3)
C68-C65-C66-C61	177.36(17)
C62-C61-C66-C65	0.1(2)
B-C61-C66-C65	172.11(16)
C64-C63-C67-F67C	147.5(2)
C62-C63-C67-F67C	-36.0(3)
C64-C63-C67-F67A	25.0(3)
C62-C63-C67-F67A	-158.5(2)
C64-C63-C67-F67B	-91.9(3)
C62-C63-C67-F67B	84.6(2)
C64-C65-C68-F68C	-40.4(3)
C66-C65-C68-F68C	142.5(2)
C64-C65-C68-F68A	-162.22(19)
C66-C65-C68-F68A	20.7(3)
C64-C65-C68-F68B	78.1(2)
C66-C65-C68-F68B	-98.9(2)
F71-C71-C72-C73	180.00(3)
C73#2-C71-C72-C73	0.00(2)
C71-C72-C73-C71#2	0.00(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+1,-y,-z

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 11

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 12

Table S6. Crystal data and structure refinement for $[\{CpRu(PEt_3)_2\}_2(\mu\text{-}N_2)][BAr'_4]_2 \cdot 2FPh$ - **1b**.

Identification code	manhj3fr
Empirical formula	C110 H104 B2 F50 N2 P4 Ru2
Formula weight	2751.60
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$ (no. 2)
Unit cell dimensions	a = 13.310(3) Å α = 83.76(1) deg. b = 13.702(3) Å β = 73.03(1) deg. c = 17.120(3) Å γ = 81.54(1) deg.
Volume	2946.7(11) Å^3
Z, Calculated density	1, 1.551 Mg/m^3
Absorption coefficient	0.437 mm^{-1}
F(000)	2772
Crystal size	0.8 x 0.7 x 0.4 mm, yellowish block
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 10 sec. per frame full sphere data collection, 4 x 606 frames
Theta range for data collection	1.25 to 30.00 deg.
Index ranges	-18 <= h <= 18, -18 <= k <= 19, -23 <= l <= 24
Reflections collected / unique	43201 / 16821 [R(int)= 0.020, R(sigma)= 0.024]
Completeness to theta = 30.00	97.9%
Absorption correction	semi-empiral from eqivalents (SADABS-2001)
Max. and min. transmission	1.000 and 0.906
Structure solution	direct methods (program SHELXS97)
Refinement method	full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	16821 / 0 / 816
Goodness-of-fit on F^2	0.950
Final R indices [I>2sigma(I)]	R1 = 0.0648, wR2 = 0.1614 (13390 data)
R indices (all data)	R1 = 0.0809, wR2 = 0.1796 (16821 data)
Extinction coefficient	0.0003(4)
Largest diff. peak and hole	1.624 and -1.074 e Å^{-3}

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S7. Atomic coordinates (x10^5 for Ru, P; x10^4 for B, C, N, F) and equivalent isotropic displacement parameters (Å^2 x 10^3) for $[\{CpRu(PEt_3)_2\}_2(\mu\text{-}N_2)][BAr'_4]_2 \cdot 2FPh$ - **1b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	51137(2)	40233(2)	37988(2)	43(1)
P(1)	49740(10)	54273(7)	29159(7)	61(1)
P(2)	32877(8)	39018(7)	42581(6)	51(1)
N	4996(2)	4817(2)	4726(2)	40(1)
C(1)	6809(5)	3441(6)	3491(7)	116(3)
C(2)	6342(6)	2908(5)	4127(5)	101(2)
C(3)	5647(6)	2423(4)	3992(4)	96(2)
C(4)	5617(7)	2666(6)	3170(7)	132(4)
C(5)	6433(8)	3325(6)	2855(4)	128(4)
C(11)	4582(13)	5299(7)	2019(5)	224(7)
C(12)	4970(9)	4664(6)	1460(4)	146(4)
C(13)	4019(8)	6470(5)	3327(7)	202(6)
C(14)	3662(14)	7252(8)	3027(15)	350(15)
C(15)	6199(7)	5984(7)	2611(7)	183(5)
C(16)	6397(16)	6835(13)	2200(11)	349(15)
C(21)	2528(5)	3914(6)	3524(4)	108(2)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 13

C(22)		2886(7)	2997(8)	3001(5)	154(4)
C(23)		2945(5)	2786(4)	4891(4)	92(2)
C(24)		3193(7)	2683(7)	5683(4)	148(4)
C(25)		2498(4)	4882(4)	4913(4)	92(2)
C(26)		1325(4)	4842(5)	5260(4)	100(2)
B		8197(2)	9920(2)	7996(2)	30(1)
C(31)		9292(2)	9550(2)	7305(2)	31(1)
C(32)		10255(2)	9784(2)	7373(2)	33(1)
C(33)		11222(2)	9491(2)	6828(2)	36(1)
C(34)		11276(2)	8941(2)	6181(2)	42(1)
C(35)		10345(2)	8684(2)	6110(2)	41(1)
C(36)		9375(2)	8971(2)	6665(2)	37(1)
C(37)		12209(3)	9751(3)	6960(2)	52(1)
C(38)		10386(3)	8108(3)	5404(3)	61(1)
C(41)		8181(2)	9122(2)	8781(2)	32(1)
C(42)		7769(2)	8223(2)	8832(2)	38(1)
C(43)		7820(3)	7488(2)	9446(2)	42(1)
C(44)		8294(3)	7613(2)	10041(2)	44(1)
C(45)		8712(2)	8488(2)	10002(2)	40(1)
C(46)		8653(2)	9228(2)	9391(2)	35(1)
C(47)		7349(4)	6555(3)	9468(3)	60(1)
C(48)		9252(3)	8631(3)	10627(2)	57(1)
C(51)		8208(2)	11070(2)	8181(2)	33(1)
C(52)		7603(2)	11483(2)	8904(2)	42(1)
C(53)		7547(3)	12489(3)	9012(2)	51(1)
C(54)		8113(3)	13112(3)	8416(2)	53(1)
C(55)		8709(3)	12724(2)	7698(2)	48(1)
C(56)		8746(2)	11728(2)	7579(2)	40(1)
C(57)		6852(4)	12885(4)	9788(3)	78(1)
C(58)		9349(4)	13359(3)	7029(3)	72(1)
C(61)		7105(2)	9958(2)	7726(2)	32(1)
C(62)		7033(2)	10113(2)	6928(2)	35(1)
C(63)		6066(2)	10204(2)	6748(2)	41(1)
C(64)		5125(2)	10180(3)	7357(2)	49(1)
C(65)		5171(2)	10071(3)	8157(2)	49(1)
C(66)		6136(2)	9947(3)	8335(2)	42(1)
C(67)		6050(3)	10331(3)	5878(2)	57(1)
C(68)		4167(3)	10125(5)	8840(3)	84(2)
F(37A)	§	13046(2)	9642(2)	6315(2)	76(1)
F(37B)		12110(2)	10651(2)	7191(2)	83(1)
F(37C)		12494(2)	9165(3)	7560(2)	93(1)
F(38A)		11257(3)	7465(4)	5202(3)	111(2)
F(38B)		9629(3)	7567(4)	5535(3)	117(2)
F(38C)		10415(7)	8669(4)	4738(2)	159(3)
F(38D)		9546(16)	8408(16)	5108(13)	61(6)
F(38E)		11122(15)	8180(16)	4800(12)	56(5)
F(38F)		10380(30)	7260(20)	5573(16)	86(8)
F(47A)		7429(8)	5920(4)	10076(4)	136(3)
F(47B)		6356(4)	6708(4)	9533(8)	188(5)
F(47C)		7742(6)	6083(4)	8815(4)	155(4)
F(47D)		6746(12)	6573(10)	9054(7)	52(4)
F(47E)		8069(13)	5798(12)	9382(14)	81(5)
F(47F)		6718(14)	6335(14)	10143(10)	71(5)
F(48A)		8965(4)	8062(3)	11301(2)	120(2)
F(48B)		9065(2)	9548(2)	10864(2)	76(1)
F(48C)		10299(2)	8492(3)	10333(2)	100(1)
F(57A)		6883(4)	13847(3)	9816(3)	153(2)
F(57B)		5868(3)	12765(4)	9919(3)	151(2)
F(57C)		7109(4)	12464(3)	10440(2)	120(1)
F(58A)		9093(4)	14314(2)	7123(3)	117(1)
F(58B)		10346(3)	13228(3)	7001(3)	157(2)
F(58C)		9261(5)	13250(3)	6325(2)	172(3)
F(67A)		6535(6)	11036(6)	5457(2)	99(2)
F(67B)		5143(5)	10576(13)	5764(4)	199(6)
F(67C)		6500(16)	9638(5)	5469(5)	258(8)
F(67D)		5546(17)	9680(16)	5711(8)	99(2)
F(67E)		6968(13)	10040(30)	5368(10)	199(6)
F(67F)		5560(50)	11134(14)	5730(14)	258(8)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 14

F(68A)	3440(4)	9723(10)	8718(3)	209(6)
F(68B)	4256(3)	9723(7)	9515(2)	157(4)
F(68C)	3765(9)	11050(8)	8955(10)	339(10)
F(68D)	4155(11)	10764(10)	9377(8)	57(4)
F(68E)	3406(10)	10564(9)	8577(7)	48(3)
F(68F)	3956(18)	9290(16)	9105(15)	111(7)
C(1S) §	9626(6)	3774(6)	2192(4)	106(2)
C(2S)	9435(4)	2958(4)	1951(4)	82(1)
C(3S)	9050(5)	3022(5)	1306(4)	92(2)
C(4S)	8886(7)	3886(8)	900(5)	127(3)
C(5S)	9079(8)	4718(7)	1160(8)	164(5)
C(6S)	9440(8)	4688(6)	1813(8)	161(4)
F(1S)	10031(8)	3709(6)	2834(5)	233(4)

Remarks: §) Four of the eight independent CF_3 groups showed significant orientation disorder and were refined with fluorine positions splitted into two sets of each three F positions of which those predominately occupied were refined with anisotropic temperature factors whereas the subordinately occupied ones were refined with isotropic temperature factors (except C(67)F_3). Refined site occupation factors for the predominately (A,B,C)/subordinately (D,E,F) sets of F sites were: F(38#) 0.87(1)/0.13(1), F(47#) 0.80(1)/0.20(1), F(67#) 0.72(1)/0.28(1), F(68#) 0.80(1)/0.20(1).
$ ordered fluorobenzene solvent molecule.

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[\{CpRu(PEt_3)_2\}_2(\mu\text{-}N_2)][BAr'_4]_2 \cdot 2FPh$ - **1b**.

	x	y	z	U_{eq}
H(1)	7392	3829	3460	139
H(2)	6506	2863	4658	121
H(3)	5237	1942	4384	115
H(4)	5239	2360	2859	159
H(5)	6706	3583	2280	154
H(11A)	3827	5225	2221	269
H(11B)	4624	5949	1717	269
H(12A)	4550	4754	1075	219
H(12B)	4955	3997	1717	219
H(12C)	5695	4767	1172	219
H(13A)	3385	6162	3630	242
H(13B)	4293	6681	3746	242
H(14A)	3221	7655	3461	525
H(14B)	3241	7114	2684	525
H(14C)	4241	7604	2698	525
H(15A)	6386	6012	3120	219
H(15B)	6729	5490	2298	219
H(16A)	7134	6917	2114	523
H(16B)	5949	7369	2509	523
H(16C)	6254	6849	1675	523
H(21A)	1775	3924	3820	129
H(21B)	2612	4518	3160	129
H(22A)	2459	3028	2624	230
H(22B)	2799	2398	3358	230
H(22C)	3625	2996	2693	230
H(23A)	2184	2762	4996	110
H(23B)	3316	2215	4581	110
H(24A)	2972	2071	5980	221
H(24B)	2820	3237	6001	221
H(24C)	3949	2674	5588	221
H(25A)	2796	4882	5374	110
H(25B)	2598	5517	4596	110
H(26A)	1009	5412	5575	150
H(26B)	1204	4241	5612	150
H(26C)	1008	4846	4816	150
H(32)	10243	10155	7808	40
H(34)	11927	8749	5803	50

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 15

H(36)	8759	8768	6605	44
H(42)	7446	8117	8433	45
H(44)	8331	7117	10460	52
H(46)	8939	9817	9387	42
H(52)	7220	11075	9331	51
H(54)	8091	13783	8498	63
H(56)	9149	11490	7072	48
H(62)	7655	10157	6496	42
H(64)	4476	10235	7231	59
H(66)	6141	9852	8886	50
H(2S)	9567	2342	2227	98
H(3S)	8892	2447	1137	110
H(4S)	8638	3918	435	153
H(5S)	8956	5330	875	197
H(6S)	9560	5266	2003	193

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for [{CpRu(PEt_3)$_2$}$_2$(μ-N_2)][BAr'$_4$]$_2$·2FPh - **1b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	48(1)	36(1)	45(1)	-4(1)	-16(1)	2(1)
P(1)	74(1)	45(1)	57(1)	8(1)	-12(1)	-2(1)
P(2)	53(1)	51(1)	55(1)	2(1)	-21(1)	-18(1)
N	34(1)	39(1)	47(1)	-1(1)	-16(1)	-3(1)
C(1)	54(3)	94(5)	177(8)	-30(5)	-5(4)	21(3)
C(2)	110(5)	80(4)	117(5)	-30(4)	-61(4)	48(4)
C(3)	114(5)	45(2)	107(4)	-2(3)	-16(4)	23(3)
C(4)	128(6)	104(5)	202(9)	-113(6)	-110(6)	75(4)
C(5)	157(7)	110(5)	58(3)	-5(3)	14(4)	83(5)
C(11)	490(20)	120(7)	105(6)	40(5)	-161(11)	-52(10)
C(12)	252(11)	125(6)	58(3)	-5(4)	-38(5)	-30(7)
C(13)	152(7)	69(4)	271(12)	79(6)	65(8)	31(4)
C(14)	330(20)	116(8)	730(40)	-182(16)	-350(30)	101(11)
C(15)	123(6)	116(6)	246(12)	77(7)	27(7)	-43(5)
C(16)	400(30)	289(19)	272(18)	-124(16)	167(18)	-240(20)
C(21)	84(4)	164(7)	96(4)	27(4)	-52(3)	-51(4)
C(22)	150(7)	249(11)	100(5)	-58(6)	-51(5)	-80(7)
C(23)	90(4)	62(3)	109(4)	21(3)	-8(3)	-20(3)
C(24)	133(6)	189(9)	87(5)	59(5)	-14(4)	6(6)
C(25)	53(2)	69(3)	140(5)	-27(3)	-1(3)	-7(2)
C(26)	53(3)	99(4)	128(5)	-3(4)	3(3)	-8(3)
B	27(1)	38(1)	26(1)	-3(1)	-7(1)	-6(1)
C(31)	29(1)	36(1)	29(1)	-2(1)	-7(1)	-6(1)
C(32)	29(1)	40(1)	31(1)	-6(1)	-7(1)	-4(1)
C(33)	29(1)	43(1)	36(1)	-7(1)	-6(1)	-4(1)
C(34)	33(1)	47(2)	40(1)	-12(1)	-1(1)	-4(1)
C(35)	41(1)	45(2)	37(1)	-13(1)	-7(1)	-5(1)
C(36)	33(1)	41(1)	37(1)	-9(1)	-8(1)	-8(1)
C(37)	32(1)	66(2)	58(2)	-21(2)	-7(1)	-6(1)
C(38)	57(2)	74(3)	54(2)	-33(2)	-9(2)	-9(2)
C(41)	28(1)	39(1)	29(1)	-3(1)	-9(1)	-5(1)
C(42)	41(1)	43(1)	35(1)	-1(1)	-16(1)	-11(1)
C(43)	45(2)	44(2)	41(2)	3(1)	-16(1)	-13(1)
C(44)	46(2)	50(2)	37(1)	7(1)	-17(1)	-8(1)
C(45)	38(1)	53(2)	33(1)	1(1)	-16(1)	-9(1)
C(46)	32(1)	45(1)	32(1)	-2(1)	-11(1)	-8(1)
C(47)	76(3)	53(2)	62(2)	10(2)	-31(2)	-27(2)
C(48)	63(2)	74(2)	46(2)	6(2)	-33(2)	-18(2)
C(51)	28(1)	38(1)	34(1)	-3(1)	-10(1)	-3(1)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 16

C(52)	36(1)	47(2)	42(2)	-11(1)	-7(1)	-4(1)
C(53)	45(2)	53(2)	56(2)	-20(2)	-14(1)	3(1)
C(54)	55(2)	39(2)	70(2)	-11(2)	-27(2)	0(1)
C(55)	50(2)	39(2)	57(2)	3(1)	-20(2)	-8(1)
C(56)	41(1)	40(1)	40(1)	-1(1)	-12(1)	-6(1)
C(57)	79(3)	72(3)	77(3)	-39(2)	-2(2)	-1(2)
C(58)	91(3)	46(2)	76(3)	8(2)	-16(2)	-21(2)
C(61)	28(1)	40(1)	28(1)	0(1)	-9(1)	-7(1)
C(62)	35(1)	42(1)	29(1)	4(1)	-10(1)	-10(1)
C(63)	46(2)	50(2)	34(1)	9(1)	-20(1)	-14(1)
C(64)	35(1)	69(2)	50(2)	9(2)	-23(1)	-15(1)
C(65)	29(1)	77(2)	40(2)	6(2)	-10(1)	-13(1)
C(66)	30(1)	65(2)	29(1)	3(1)	-8(1)	-9(1)
C(67)	67(2)	70(2)	45(2)	13(2)	-32(2)	-19(2)
C(68)	36(2)	137(5)	69(3)	12(3)	-6(2)	-13(2)
F(37A)	32(1)	117(2)	75(2)	-36(2)	4(1)	-18(1)
F(37B)	45(1)	83(2)	125(2)	-52(2)	-11(1)	-17(1)
F(37C)	66(2)	135(3)	93(2)	9(2)	-50(2)	-20(2)
F(38A)	81(2)	132(4)	134(4)	-103(3)	-36(2)	28(2)
F(38B)	85(3)	171(5)	108(3)	-94(3)	7(2)	-61(3)
F(38C)	349(10)	96(3)	55(2)	-13(2)	-87(4)	-27(5)
F(47A)	247(9)	77(3)	142(5)	62(3)	-133(6)	-92(4)
F(47B)	57(3)	74(3)	435(14)	-13(5)	-60(5)	-33(2)
F(47C)	231(7)	112(4)	112(4)	-57(3)	32(4)	-114(5)
F(48A)	198(4)	136(3)	70(2)	48(2)	-92(2)	-91(3)
F(48B)	88(2)	93(2)	63(1)	-24(1)	-42(1)	-11(1)
F(48C)	61(2)	149(3)	111(2)	-50(2)	-57(2)	14(2)
F(57A)	205(5)	78(2)	133(3)	-63(2)	40(3)	-17(3)
F(57B)	58(2)	228(5)	155(4)	-120(4)	17(2)	0(2)
F(57C)	141(3)	144(3)	62(2)	-42(2)	-2(2)	-5(3)
F(58A)	157(3)	50(2)	134(3)	21(2)	-26(3)	-30(2)
F(58B)	74(2)	146(4)	206(5)	96(4)	-1(3)	-29(2)
F(58C)	337(8)	140(3)	61(2)	28(2)	-41(3)	-156(5)
F(67A)	140(4)	130(4)	41(2)	31(2)	-36(2)	-72(4)
F(67B)	77(3)	472(18)	67(3)	90(6)	-54(3)	-103(6)
F(67C)	630(20)	75(3)	83(5)	-36(3)	-181(10)	80(8)
F(67D)	140(4)	130(4)	41(2)	31(2)	-36(2)	-72(4)
F(67E)	77(3)	472(18)	67(3)	90(6)	-54(3)	-103(6)
F(67F)	630(20)	75(3)	83(5)	-36(3)	-181(10)	80(8)
F(68A)	73(3)	509(18)	71(3)	6(5)	-10(2)	-157(6)
F(68B)	45(2)	381(12)	37(2)	18(3)	2(1)	-52(4)
F(68C)	211(10)	183(9)	391(17)	17(10)	218(11)	67(8)
C(1S)	108(5)	128(6)	95(4)	0(4)	-45(4)	-23(4)
C(2S)	71(3)	71(3)	88(4)	10(3)	-10(3)	0(2)
C(3S)	84(4)	92(4)	90(4)	-24(3)	-3(3)	-13(3)
C(4S)	130(6)	152(8)	119(6)	24(5)	-69(5)	-34(6)
C(5S)	166(9)	94(5)	261(13)	70(7)	-127(9)	-28(5)
C(6S)	170(9)	72(4)	278(14)	-10(6)	-116(9)	-27(5)
F(1S)	339(11)	229(7)	200(7)	28(6)	-166(7)	-98(7)

Table S10. Bond lengths [Å] and angles [deg] for $[\{CpRu(PEt_3)_2\}_2(\mu\text{-}N_2)][BAr'_4]_2 \cdot 2FPh$ - **1b.**

Bond distances

Ru-N	1.977(3)	P(1)-C(15)	1.815(8)
Ru-C(4)	2.171(5)	P(1)-C(13)	1.821(8)
Ru-C(5)	2.190(5)		
Ru-C(1)	2.208(5)	P(2)-C(23)	1.810(5)
Ru-C(2)	2.222(5)	P(2)-C(21)	1.827(5)
Ru-C(3)	2.223(5)	P(2)-C(25)	1.841(5)
Ru-P(1)	2.3339(11)		
Ru-P(2)	2.3512(11)	N-N#1	1.114(5)
		C(1)-C(2)	1.293(10)
P(1)-C(11)	1.793(9)	C(1)-C(5)	1.356(12)
		C(1)-H(1)	0.99

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 17

C(2)-C(3)	1.299(10)
C(2)-H(2)	0.99
C(3)-C(4)	1.420(11)
C(3)-H(3)	0.99
C(4)-C(5)	1.458(12)
C(4)-H(4)	0.99
C(5)-H(5)	0.99
C(11)-C(12)	1.305(12)
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(12)-H(12A)	0.97
C(12)-H(12B)	0.97
C(12)-H(12C)	0.97
C(13)-C(14)	1.230(15)
C(13)-H(13A)	0.98
C(13)-H(13B)	0.98
C(14)-H(14A)	0.97
C(14)-H(14B)	0.97
C(14)-H(14C)	0.97
C(15)-C(16)	1.314(17)
C(15)-H(15A)	0.98
C(15)-H(15B)	0.98
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
C(16)-H(16C)	0.97
C(21)-C(22)	1.557(11)
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(22)-H(22A)	0.97
C(22)-H(22B)	0.97
C(22)-H(22C)	0.97
C(23)-C(24)	1.474(10)
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(24)-H(24A)	0.97
C(24)-H(24B)	0.97
C(24)-H(24C)	0.97
C(25)-C(26)	1.506(7)
C(25)-H(25A)	0.98
C(25)-H(25B)	0.98
C(26)-H(26A)	0.97
C(26)-H(26B)	0.97
C(26)-H(26C)	0.97
B-C(41)	1.635(4)
B-C(31)	1.639(4)
B-C(61)	1.641(4)
B-C(51)	1.644(4)
C(31)-C(36)	1.391(4)
C(31)-C(32)	1.406(4)
C(32)-C(33)	1.384(4)
C(32)-H(32)	0.94
C(33)-C(34)	1.385(4)
C(33)-C(37)	1.494(4)
C(34)-C(35)	1.379(4)
C(34)-H(34)	0.94
C(35)-C(36)	1.393(4)
C(35)-C(38)	1.497(4)
C(36)-H(36)	0.94
C(37)-F(37B)	1.313(4)
C(37)-F(37A)	1.322(4)
C(37)-F(37C)	1.343(5)
C(38)-F(38F)	1.17(3)
C(38)-F(38E)	1.205(19)
C(38)-F(38B)	1.291(5)
C(38)-F(38C)	1.298(6)
C(38)-F(38A)	1.331(6)
C(38)-F(38D)	1.35(2)
C(41)-C(46)	1.396(4)
C(41)-C(42)	1.404(4)
C(42)-C(43)	1.383(4)
C(42)-H(42)	0.94
C(43)-C(44)	1.383(4)
C(43)-C(47)	1.497(5)
C(44)-C(45)	1.382(5)
C(44)-H(44)	0.94
C(45)-C(46)	1.386(4)
C(45)-C(48)	1.496(4)
C(46)-H(46)	0.94
C(47)-F(47D)	1.212(14)
C(47)-F(47F)	1.251(16)
C(47)-F(47B)	1.280(6)
C(47)-F(47E)	1.293(17)
C(47)-F(47C)	1.287(6)
C(47)-F(47A)	1.301(5)
C(48)-F(48A)	1.312(5)
C(48)-F(48C)	1.328(5)
C(48)-F(48B)	1.330(5)
C(51)-C(56)	1.395(4)
C(51)-C(52)	1.392(4)
C(52)-C(53)	1.399(5)
C(52)-H(52)	0.94
C(53)-C(54)	1.374(6)
C(53)-C(57)	1.486(5)
C(54)-C(55)	1.368(5)
C(54)-H(54)	0.94
C(55)-C(56)	1.393(4)
C(55)-C(58)	1.492(5)
C(56)-H(56)	0.94
C(57)-F(57B)	1.295(6)
C(57)-F(57C)	1.310(7)
C(57)-F(57A)	1.331(6)
C(58)-F(58C)	1.271(6)
C(58)-F(58B)	1.300(7)
C(58)-F(58A)	1.318(5)
C(61)-C(62)	1.389(4)
C(61)-C(66)	1.402(4)
C(62)-C(63)	1.394(4)
C(62)-H(62)	0.94
C(63)-C(64)	1.377(5)
C(63)-C(67)	1.487(4)
C(64)-C(65)	1.381(5)
C(64)-H(64)	0.94
C(65)-C(66)	1.387(4)
C(65)-C(68)	1.496(5)
C(66)-H(66)	0.94
C(67)-F(67C)	1.218(8)
C(67)-F(67F)	1.24(2)
C(67)-F(67A)	1.278(6)
C(67)-F(67D)	1.292(16)
C(67)-F(67B)	1.270(7)
C(67)-F(67E)	1.31(3)
C(68)-F(68F)	1.23(2)
C(68)-F(68B)	1.255(7)
C(68)-F(68E)	1.272(13)
C(68)-F(68A)	1.259(8)
C(68)-F(68C)	1.312(11)
C(68)-F(68D)	1.331(14)
C(1S)-C(2S)	1.315(9)
C(1S)-F(1S)	1.349(8)
C(1S)-C(6S)	1.369(11)
C(2S)-C(3S)	1.338(9)
C(2S)-H(2S)	0.94

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 18

C(3S)-C(4S)	1.328(10)
C(3S)-H(3S)	0.94
C(4S)-C(5S)	1.352(13)
C(4S)-H(4S)	0.94
C(5S)-C(6S)	1.334(14)
C(5S)-H(5S)	0.94
C(6S)-H(6S)	0.94

Bond angles

N-Ru-C(4)	151.6(2)
N-Ru-C(5)	134.7(4)
C(4)-Ru-C(5)	39.1(3)
N-Ru-C(1)	100.7(3)
C(4)-Ru-C(1)	61.9(3)
C(5)-Ru-C(1)	35.9(3)
N-Ru-C(2)	92.55(19)
C(4)-Ru-C(2)	60.2(2)
C(5)-Ru-C(2)	58.7(3)
C(1)-Ru-C(2)	33.9(3)
N-Ru-C(3)	114.6(2)
C(4)-Ru-C(3)	37.7(3)
C(5)-Ru-C(3)	61.4(3)
C(1)-Ru-C(3)	58.4(3)
C(2)-Ru-C(3)	34.0(2)
N-Ru-P(1)	92.68(8)
C(4)-Ru-P(1)	113.1(3)
C(5)-Ru-P(1)	90.79(17)
C(1)-Ru-P(1)	106.3(3)
C(2)-Ru-P(1)	140.0(3)
C(3)-Ru-P(1)	149.94(18)
N-Ru-P(2)	90.43(8)
C(4)-Ru-P(2)	98.3(3)
C(5)-Ru-P(2)	134.1(4)
C(1)-Ru-P(2)	155.0(2)
C(2)-Ru-P(2)	124.2(3)
C(3)-Ru-P(2)	96.6(2)
P(1)-Ru-P(2)	95.42(4)
C(11)-P(1)-C(15)	108.8(6)
C(11)-P(1)-C(13)	99.4(6)
C(15)-P(1)-C(13)	101.2(5)
C(11)-P(1)-Ru	117.9(3)
C(15)-P(1)-Ru	110.3(3)
C(13)-P(1)-Ru	117.4(3)
C(23)-P(2)-C(21)	101.2(3)
C(23)-P(2)-C(25)	102.5(3)
C(21)-P(2)-C(25)	101.2(3)
C(23)-P(2)-Ru	114.3(2)
C(21)-P(2)-Ru	120.4(2)
C(25)-P(2)-Ru	114.81(16)
N#1-N-Ru	172.3(3)
C(2)-C(1)-C(5)	109.4(8)
C(2)-C(1)-Ru	73.6(3)
C(5)-C(1)-Ru	71.3(4)
C(2)-C(1)-H(1)	125.2
C(5)-C(1)-H(1)	125.2
Ru-C(1)-H(1)	125.2
C(1)-C(2)-C(3)	113.0(7)
C(1)-C(2)-Ru	72.4(3)
C(3)-C(2)-Ru	73.1(3)
C(1)-C(2)-H(2)	123.5
C(3)-C(2)-H(2)	123.5
Ru-C(2)-H(2)	123.5
C(2)-C(3)-C(4)	108.1(7)
C(2)-C(3)-Ru	73.0(3)
C(4)-C(3)-Ru	69.1(3)
C(2)-C(3)-H(3)	125.9
C(4)-C(3)-H(3)	125.9
Ru-C(3)-H(3)	125.9
C(3)-C(4)-C(5)	103.0(6)
C(3)-C(4)-Ru	73.2(3)
C(5)-C(4)-Ru	71.2(3)
C(3)-C(4)-H(4)	128.0
C(5)-C(4)-H(4)	128.0
Ru-C(4)-H(4)	128.0
C(1)-C(5)-C(4)	106.3(6)
C(1)-C(5)-Ru	72.8(3)
C(4)-C(5)-Ru	69.8(3)
C(1)-C(5)-H(5)	126.7
C(4)-C(5)-H(5)	126.7
Ru-C(5)-H(5)	126.7
C(12)-C(11)-P(1)	129.4(10)
C(12)-C(11)-H(11A)	104.9
P(1)-C(11)-H(11A)	104.9
C(12)-C(11)-H(11B)	104.9
P(1)-C(11)-H(11B)	104.9
H(11A)-C(11)-H(11B)	105.8
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-P(1)	134.5(13)
C(14)-C(13)-H(13A)	103.6
P(1)-C(13)-H(13A)	103.6
C(14)-C(13)-H(13B)	103.6
P(1)-C(13)-H(13B)	103.6
H(13A)-C(13)-H(13B)	105.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-P(1)	128.9(13)
C(16)-C(15)-H(15A)	105.1
P(1)-C(15)-H(15A)	105.1
C(16)-C(15)-H(15B)	105.1
P(1)-C(15)-H(15B)	105.1
H(15A)-C(15)-H(15B)	105.9
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(22)-C(21)-P(2)	112.1(5)
C(22)-C(21)-H(21A)	109.2
P(2)-C(21)-H(21A)	109.2
C(22)-C(21)-H(21B)	109.2
P(2)-C(21)-H(21B)	109.2
H(21A)-C(21)-H(21B)	107.9
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-P(2)	115.5(5)
C(24)-C(23)-H(23A)	108.4
P(2)-C(23)-H(23A)	108.4
C(24)-C(23)-H(23B)	108.4
P(2)-C(23)-H(23B)	108.4
H(23A)-C(23)-H(23B)	107.5

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 19

C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-P(2)	118.4(4)
C(26)-C(25)-H(25A)	107.7
P(2)-C(25)-H(25A)	107.7
C(26)-C(25)-H(25B)	107.7
P(2)-C(25)-H(25B)	107.7
H(25A)-C(25)-H(25B)	107.1
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(41)-B-C(31)	104.1(2)
C(41)-B-C(61)	110.0(2)
C(31)-B-C(61)	115.4(2)
C(41)-B-C(51)	114.4(2)
C(31)-B-C(51)	109.6(2)
C(61)-B-C(51)	103.7(2)
C(36)-C(31)-C(32)	115.4(2)
C(36)-C(31)-B	126.0(2)
C(32)-C(31)-B	118.6(2)
C(33)-C(32)-C(31)	122.8(2)
C(33)-C(32)-H(32)	118.6
C(31)-C(32)-H(32)	118.6
C(32)-C(33)-C(34)	120.4(3)
C(32)-C(33)-C(37)	119.2(3)
C(34)-C(33)-C(37)	120.4(3)
C(35)-C(34)-C(33)	118.0(3)
C(35)-C(34)-H(34)	121.0
C(33)-C(34)-H(34)	121.0
C(34)-C(35)-C(36)	121.4(3)
C(34)-C(35)-C(38)	118.7(3)
C(36)-C(35)-C(38)	119.9(3)
C(31)-C(36)-C(35)	122.0(3)
C(31)-C(36)-H(36)	119.0
C(35)-C(36)-H(36)	119.0
F(37B)-C(37)-F(37A)	108.4(3)
F(37B)-C(37)-F(37C)	104.5(3)
F(37A)-C(37)-F(37C)	104.4(3)
F(37B)-C(37)-C(33)	113.3(3)
F(37A)-C(37)-C(33)	113.7(3)
F(37C)-C(37)-C(33)	111.9(3)
F(38B)-C(38)-F(38A)	103.6(4)
F(38C)-C(38)-F(38A)	104.1(5)
F(38B)-C(38)-F(38C)	108.6(5)
F(38F)-C(38)-F(38E)	105.1(17)
F(38F)-C(38)-F(38D)	106.5(17)
F(38E)-C(38)-F(38D)	102.3(13)
F(38A)-C(38)-C(35)	112.6(4)
F(38B)-C(38)-C(35)	114.7(3)
F(38C)-C(38)-C(35)	112.3(4)
F(38F)-C(38)-C(35)	113.4(13)
F(38E)-C(38)-C(35)	117.2(9)
F(38D)-C(38)-C(35)	111.3(9)
C(46)-C(41)-C(42)	115.7(2)
C(46)-C(41)-B	123.7(2)
C(42)-C(41)-B	120.4(2)
C(43)-C(42)-C(41)	122.6(3)
C(43)-C(42)-H(42)	118.7
C(41)-C(42)-H(42)	118.7
C(42)-C(43)-C(44)	120.5(3)
C(42)-C(43)-C(47)	119.7(3)
C(44)-C(43)-C(47)	119.9(3)
C(43)-C(44)-C(45)	118.0(3)
C(43)-C(44)-H(44)	121.0
C(45)-C(44)-H(44)	121.0
C(46)-C(45)-C(44)	121.5(3)
C(46)-C(45)-C(48)	119.5(3)
C(44)-C(45)-C(48)	119.0(3)
C(45)-C(46)-C(41)	121.7(3)
C(45)-C(46)-H(46)	119.1
C(41)-C(46)-H(46)	119.1
F(47B)-C(47)-F(47A)	104.6(6)
F(47C)-C(47)-F(47A)	106.1(6)
F(47B)-C(47)-F(47C)	103.9(7)
F(47D)-C(47)-F(47F)	97.3(11)
F(47D)-C(47)-F(47E)	114.5(11)
F(47F)-C(47)-F(47E)	102.2(12)
F(47A)-C(47)-C(43)	114.5(3)
F(47B)-C(47)-C(43)	112.8(4)
F(47C)-C(47)-C(43)	113.9(4)
F(47D)-C(47)-C(43)	116.6(7)
F(47E)-C(47)-C(43)	110.8(8)
F(47F)-C(47)-C(43)	113.9(8)
F(48A)-C(48)-F(48C)	109.1(4)
F(48A)-C(48)-F(48B)	105.4(4)
F(48C)-C(48)-F(48B)	103.1(3)
F(48A)-C(48)-C(45)	113.2(3)
F(48C)-C(48)-C(45)	112.0(3)
F(48B)-C(48)-C(45)	113.3(3)
C(56)-C(51)-C(52)	115.4(3)
C(56)-C(51)-B	121.2(2)
C(52)-C(51)-B	123.1(2)
C(51)-C(52)-C(53)	121.8(3)
C(51)-C(52)-H(52)	119.1
C(53)-C(52)-H(52)	119.1
C(54)-C(53)-C(52)	121.4(3)
C(54)-C(53)-C(57)	119.8(4)
C(52)-C(53)-C(57)	118.8(4)
C(55)-C(54)-C(53)	117.8(3)
C(55)-C(54)-H(54)	121.1
C(53)-C(54)-H(54)	121.1
C(54)-C(55)-C(56)	121.0(3)
C(54)-C(55)-C(58)	120.4(3)
C(56)-C(55)-C(58)	118.5(3)
C(51)-C(56)-C(55)	122.6(3)
C(51)-C(56)-H(56)	118.7
C(55)-C(56)-H(56)	118.7
F(57B)-C(57)-F(57C)	105.0(5)
F(57B)-C(57)-F(57A)	106.8(5)
F(57C)-C(57)-F(57A)	105.2(5)
F(57B)-C(57)-C(53)	113.2(4)
F(57C)-C(57)-C(53)	113.4(4)
F(57A)-C(57)-C(53)	112.6(5)
F(58C)-C(58)-F(58B)	108.9(6)
F(58C)-C(58)-F(58A)	104.6(5)
F(58B)-C(58)-F(58A)	102.6(4)
F(58C)-C(58)-C(55)	113.6(4)
F(58B)-C(58)-C(55)	112.4(4)
F(58A)-C(58)-C(55)	113.7(4)
C(62)-C(61)-C(66)	115.3(2)
C(62)-C(61)-B	125.1(2)
C(66)-C(61)-B	119.2(2)
C(61)-C(62)-C(63)	121.9(3)
C(61)-C(62)-H(62)	119.0
C(63)-C(62)-H(62)	119.0
C(64)-C(63)-C(62)	121.7(3)
C(64)-C(63)-C(67)	119.2(3)
C(62)-C(63)-C(67)	119.1(3)
C(65)-C(64)-C(63)	117.5(3)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 20

C(65)-C(64)-H(64)	121.3
C(63)-C(64)-H(64)	121.3
C(64)-C(65)-C(66)	120.8(3)
C(64)-C(65)-C(68)	119.6(3)
C(66)-C(65)-C(68)	119.6(3)
C(65)-C(66)-C(61)	122.7(3)
C(65)-C(66)-H(66)	118.6
C(61)-C(66)-H(66)	118.6
F(67A)-C(67)-F(67B)	100.0(6)
F(67C)-C(67)-F(67A)	100.7(8)
F(67C)-C(67)-F(67B)	108.9(8)
F(67F)-C(67)-F(67D)	104(2)
F(67F)-C(67)-F(67E)	119(2)
F(67D)-C(67)-F(67E)	95.7(16)
F(67C)-C(67)-C(63)	115.1(4)
F(67F)-C(67)-C(63)	111.2(8)
F(67A)-C(67)-C(63)	114.8(3)
F(67D)-C(67)-C(63)	111.5(6)
F(67B)-C(67)-C(63)	115.4(4)
F(67E)-C(67)-C(63)	112.9(7)
F(68B)-C(68)-F(68A)	103.7(6)
F(68A)-C(68)-F(68C)	104.8(9)
F(68B)-C(68)-F(68C)	107.5(10)
F(68F)-C(68)-F(68E)	107.7(13)
F(68E)-C(68)-F(68D)	98.6(9)
F(68F)-C(68)-F(68D)	117.9(13)
F(68F)-C(68)-C(65)	110.1(11)
F(68B)-C(68)-C(65)	115.0(4)
F(68E)-C(68)-C(65)	109.8(7)
F(68A)-C(68)-C(65)	114.6(6)
F(68C)-C(68)-C(65)	110.5(5)
F(68D)-C(68)-C(65)	111.9(7)
C(2S)-C(1S)-F(1S)	118.7(7)
C(2S)-C(1S)-C(6S)	122.8(7)
F(1S)-C(1S)-C(6S)	118.6(8)
C(1S)-C(2S)-C(3S)	118.6(6)
C(1S)-C(2S)-H(2S)	120.7
C(3S)-C(2S)-H(2S)	120.7
C(4S)-C(3S)-C(2S)	121.1(7)
C(4S)-C(3S)-H(3S)	119.4
C(2S)-C(3S)-H(3S)	119.4
C(3S)-C(4S)-C(5S)	119.4(8)
C(3S)-C(4S)-H(4S)	120.3
C(5S)-C(4S)-H(4S)	120.3
C(6S)-C(5S)-C(4S)	121.2(7)
C(6S)-C(5S)-H(5S)	119.4
C(4S)-C(5S)-H(5S)	119.4
C(5S)-C(6S)-C(1S)	116.8(8)
C(5S)-C(6S)-H(6S)	121.6
C(1S)-C(6S)-H(6S)	121.6

Torsion angles

N-Ru-P1-C11	-159.6(6)
C4-Ru-P1-C11	32.6(6)
C5-Ru-P1-C11	65.6(7)
C1-Ru-P1-C11	98.4(7)
C2-Ru-P1-C11	103.2(7)
C3-Ru-P1-C11	44.3(7)
P2-Ru-P1-C11	-68.9(6)
N-Ru-P1-C15	74.6(4)
C4-Ru-P1-C15	-93.3(5)
C5-Ru-P1-C15	-60.3(6)
C1-Ru-P1-C15	-27.4(5)
C2-Ru-P1-C15	-22.6(5)
C3-Ru-P1-C15	-81.6(6)
P2-Ru-P1-C15	165.2(4)
N-Ru-P1-C13	-40.7(5)
C4-Ru-P1-C13	151.5(6)
C5-Ru-P1-C13	-175.5(6)
C1-Ru-P1-C13	-142.6(6)
C2-Ru-P1-C13	-137.9(6)
C3-Ru-P1-C13	163.2(7)
P2-Ru-P1-C13	50.0(5)
N-Ru-P2-C23	-95.2(3)
C4-Ru-P2-C23	57.7(4)
C5-Ru-P2-C23	75.7(3)
C1-Ru-P2-C23	21.8(7)
C2-Ru-P2-C23	-1.8(3)
C3-Ru-P2-C23	19.7(3)
P1-Ru-P2-C23	172.1(2)
N-Ru-P2-C21	144.1(3)
C4-Ru-P2-C21	-63.0(4)
C5-Ru-P2-C21	-45.0(4)
C1-Ru-P2-C21	-98.9(7)
C2-Ru-P2-C21	-122.5(4)
C3-Ru-P2-C21	-101.0(4)
P1-Ru-P2-C21	51.4(3)
N-Ru-P2-C25	22.9(3)
C4-Ru-P2-C25	175.7(4)
C5-Ru-P2-C25	-166.3(3)
C1-Ru-P2-C25	139.9(7)
C2-Ru-P2-C25	116.2(3)
C3-Ru-P2-C25	137.7(3)
P1-Ru-P2-C25	-69.9(3)
C4-Ru-N-N#1	10(3)
C5-Ru-N-N#1	-52(3)
C1-Ru-N-N#1	-39(3)
C2-Ru-N-N#1	-5(3)
C3-Ru-N-N#1	21(3)
P1-Ru-N-N#1	-146(3)
P2-Ru-N-N#1	119(3)
N-Ru-C1-C2	78.5(5)
C4-Ru-C1-C2	-77.5(5)
C5-Ru-C1-C2	-117.7(7)
C3-Ru-C1-C2	-34.0(4)
P1-Ru-C1-C2	174.5(4)
P2-Ru-C1-C2	-36.5(10)
N-Ru-C1-C5	-163.8(5)
C4-Ru-C1-C5	40.2(5)
C2-Ru-C1-C5	117.7(7)
C3-Ru-C1-C5	83.8(5)
P1-Ru-C1-C5	-67.8(6)
P2-Ru-C1-C5	81.3(10)
C5-C1-C2-C3	-0.6(7)
Ru-C1-C2-C3	62.2(4)
C5-C1-C2-Ru	-62.8(4)
N-Ru-C2-C1	-105.4(5)
C4-Ru-C2-C1	83.1(6)
C5-Ru-C2-C1	37.4(5)
C3-Ru-C2-C1	121.7(7)
P1-Ru-C2-C1	-8.2(7)
P2-Ru-C2-C1	162.3(5)
N-Ru-C2-C3	132.9(5)
C4-Ru-C2-C3	-38.6(5)
C5-Ru-C2-C3	-84.2(5)
C1-Ru-C2-C3	-121.7(7)
P1-Ru-C2-C3	-129.9(5)
P2-Ru-C2-C3	40.6(5)
C1-C2-C3-C4	-1.3(7)
Ru-C2-C3-C4	60.5(4)
C1-C2-C3-Ru	-61.8(4)
N-Ru-C3-C2	-53.6(5)
C4-Ru-C3-C2	117.7(7)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 21

C5-Ru-C3-C2	75.5(6)
C1-Ru-C3-C2	33.9(5)
P1-Ru-C3-C2	99.9(6)
P2-Ru-C3-C2	-147.2(5)
N-Ru-C3-C4	-171.4(5)
C5-Ru-C3-C4	-42.2(5)
C1-Ru-C3-C4	-83.8(5)
C2-Ru-C3-C4	-117.7(7)
P1-Ru-C3-C4	-17.8(8)
P2-Ru-C3-C4	95.1(5)
C2-C3-C4-C5	2.5(6)
Ru-C3-C4-C5	65.4(3)
C2-C3-C4-Ru	-62.9(4)
N-Ru-C4-C3	16.7(10)
C5-Ru-C4-C3	110.6(6)
C1-Ru-C4-C3	73.7(5)
C2-Ru-C4-C3	34.8(4)
P1-Ru-C4-C3	170.4(4)
P2-Ru-C4-C3	-90.0(5)
N-Ru-C4-C5	-94.0(9)
C1-Ru-C4-C5	-36.9(4)
C2-Ru-C4-C5	-75.9(5)
C3-Ru-C4-C5	-110.6(6)
P1-Ru-C4-C5	59.8(5)
P2-Ru-C4-C5	159.4(5)
C2-C1-C5-C4	2.2(6)
Ru-C1-C5-C4	-62.1(4)
C2-C1-C5-Ru	64.2(4)
C3-C4-C5-C1	-2.8(6)
Ru-C4-C5-C1	64.1(4)
C3-C4-C5-Ru	-66.8(3)
N-Ru-C5-C1	22.7(7)
C4-Ru-C5-C1	-115.3(6)
C2-Ru-C5-C1	-35.3(4)
C3-Ru-C5-C1	-74.7(5)
P1-Ru-C5-C1	117.3(6)
P2-Ru-C5-C1	-144.4(5)
N-Ru-C5-C4	138.1(5)
C1-Ru-C5-C4	115.3(6)
C2-Ru-C5-C4	80.0(5)
C3-Ru-C5-C4	40.7(4)
P1-Ru-C5-C4	-127.4(5)
P2-Ru-C5-C4	-29.0(6)
C15-P1-C11-C12	75.0(13)
C13-P1-C11-C12	-179.6(12)
Ru-P1-C11-C12	-51.5(15)
C11-P1-C13-C14	-41.9(17)
C15-P1-C13-C14	69.6(17)
Ru-P1-C13-C14	-170.3(15)
C11-P1-C15-C16	57.8(15)
C13-P1-C15-C16	-46.3(15)
Ru-P1-C15-C16	-171.4(13)
C23-P2-C21-C22	-62.5(6)
C25-P2-C21-C22	-167.8(5)
Ru-P2-C21-C22	64.5(6)
C21-P2-C23-C24	-164.2(6)
C25-P2-C23-C24	-59.9(6)
Ru-P2-C23-C24	64.9(6)
C23-P2-C25-C26	-53.3(6)
C21-P2-C25-C26	50.9(6)
Ru-P2-C25-C26	-177.9(5)
C41-B-C31-C36	97.5(3)
C61-B-C31-C36	-23.2(4)
C51-B-C31-C36	-139.7(3)
C41-B-C31-C32	-78.9(3)
C61-B-C31-C32	160.4(2)
C51-B-C31-C32	43.8(3)
C36-C31-C32-C33	2.1(4)
B-C31-C32-C33	178.9(3)
C31-C32-C33-C34	-0.2(5)
C31-C32-C33-C37	-178.5(3)
C32-C33-C34-C35	-1.2(5)
C37-C33-C34-C35	177.1(3)
C33-C34-C35-C36	0.5(5)
C33-C34-C35-C38	178.7(3)
C32-C31-C36-C35	-2.8(4)
B-C31-C36-C35	-179.3(3)
C34-C35-C36-C31	1.6(5)
C38-C35-C36-C31	-176.6(3)
C32-C33-C37-F37B	-40.9(5)
C34-C33-C37-F37B	140.8(3)
C32-C33-C37-F37A	-165.2(3)
C34-C33-C37-F37A	16.5(5)
C32-C33-C37-F37C	76.9(4)
C34-C33-C37-F37C	-101.4(4)
C34-C35-C38-F38F	98.2(18)
C36-C35-C38-F38F	-83.6(18)
C34-C35-C38-F38E	-24.6(14)
C36-C35-C38-F38E	153.6(13)
C34-C35-C38-F38B	153.5(5)
C36-C35-C38-F38B	-28.3(6)
C34-C35-C38-F38C	-81.9(6)
C36-C35-C38-F38C	96.3(6)
C34-C35-C38-F38A	35.3(6)
C36-C35-C38-F38A	-146.5(4)
C34-C35-C38-F38B	-141.8(11)
C36-C35-C38-F38B	36.4(12)
C31-B-C41-C46	88.4(3)
C61-B-C41-C46	-147.4(3)
C51-B-C41-C46	-31.2(3)
C31-B-C41-C42	-85.2(3)
C61-B-C41-C42	39.1(3)
C51-B-C41-C42	155.2(2)
C46-C41-C42-C43	0.3(4)
B-C41-C42-C43	174.3(3)
C41-C42-C43-C44	-0.4(5)
C41-C42-C43-C47	179.1(3)
C42-C43-C44-C45	0.0(5)
C47-C43-C44-C45	-179.5(3)
C43-C44-C45-C46	0.6(5)
C43-C44-C45-C48	-178.5(3)
C44-C45-C46-C41	-0.7(5)
C48-C45-C46-C41	178.4(3)
C42-C41-C46-C45	0.3(4)
B-C41-C46-C45	-173.5(3)
C42-C43-C47-F47D	-15.6(9)
C44-C43-C47-F47D	163.9(8)
C42-C43-C47-F47F	-127.7(12)
C44-C43-C47-F47F	51.8(12)
C42-C43-C47-F47B	-59.7(8)
C44-C43-C47-F47B	119.8(8)
C42-C43-C47-F47E	117.8(11)
C44-C43-C47-F47E	-62.7(12)
C42-C43-C47-F47C	58.4(7)
C44-C43-C47-F47C	-122.1(6)
C42-C43-C47-F47A	-179.2(6)
C44-C43-C47-F47A	0.3(8)
C46-C45-C48-F481	158.9(4)
C44-C45-C48-F48A	-22.0(5)
C46-C45-C48-F48C	-77.3(5)
C44-C45-C48-F48C	101.8(4)
C46-C45-C48-F48B	38.9(5)
C44-C45-C48-F48B	-142.0(3)
C41-B-C51-C56	146.2(3)
C31-B-C51-C56	29.7(3)
C61-B-C51-C56	-94.0(3)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 22

C41-B-C51-C52	-40.9(3)	C63-C64-C65-C66	-2.9(6)
C31-B-C51-C52	-157.4(3)	C63-C64-C65-C68	174.9(4)
C61-B-C51-C52	78.9(3)	C64-C65-C66-C61	2.2(6)
C56-C51-C52-C53	-0.3(4)	C68-C65-C66-C61	-175.6(4)
B-C51-C52-C53	-173.6(3)	C62-C61-C66-C65	0.7(5)
C51-C52-C53-C54	-1.7(5)	B-C61-C66-C65	173.7(3)
C51-C52-C53-C57	177.7(4)	C64-C63-C67-F67C	-116.7(11)
C52-C53-C54-C55	2.1(5)	C62-C63-C67-F67C	63.3(12)
C57-C53-C54-C55	-177.4(4)	C64-C63-C67-F67F	62(3)
C53-C54-C55-C56	-0.4(5)	C62-C63-C67-F67F	-118(3)
C53-C54-C55-C58	-179.4(4)	C64-C63-C67-F67A	127.1(6)
C52-C51-C56-C55	2.0(4)	C62-C63-C67-F67A	-52.9(7)
B-C51-C56-C55	175.4(3)	C64-C63-C67-F67D	-53.6(14)
C54-C55-C56-C51	-1.7(5)	C62-C63-C67-F67D	126.4(13)
C58-C55-C56-C51	177.3(3)	C64-C63-C67-F67B	11.6(10)
C54-C53-C57-F57B	120.0(5)	C62-C63-C67-F67B	-168.5(9)
C52-C53-C57-F57B	-59.5(7)	C64-C63-C67-F67E	-160(2)
C54-C53-C57-F57C	-120.6(5)	C62-C63-C67-F67E	20(2)
C52-C53-C57-F57C	60.0(6)	C64-C65-C68-F68F	98.3(15)
C54-C53-C57-F57A	-1.3(7)	C66-C65-C68-F68F	-83.8(15)
C52-C53-C57-F57A	179.2(5)	C64-C65-C68-F68B	158.5(6)
C54-C55-C58-F58C	-134.3(5)	C66-C65-C68-F68B	-23.7(9)
C56-C55-C58-F58C	46.7(6)	C64-C65-C68-F68E	-20.0(9)
C54-C55-C58-F58B	101.4(5)	C66-C65-C68-F68E	157.8(7)
C56-C55-C58-F58B	-77.6(6)	C64-C65-C68-F68A	38.5(10)
C54-C55-C58-F58A	-14.7(6)	C66-C65-C68-F68A	-143.7(8)
C56-C55-C58-F58A	166.3(4)	C64-C65-C68-F68C	-79.6(12)
C41-B-C61-C62	-145.6(3)	C66-C65-C68-F68C	98.2(11)
C31-B-C61-C62	-28.2(4)	C64-C65-C68-F68D	-128.5(8)
C51-B-C61-C62	91.7(3)	C66-C65-C68-F68D	49.3(9)
C41-B-C61-C66	42.1(3)	F1S-C1S-C2S-C3S	-179.0(7)
C31-B-C61-C66	159.5(3)	C6S-C1S-C2S-C3S	0.5(12)
C51-B-C61-C66	-80.6(3)	C1S-C2S-C3S-C4S	1.7(10)
C66-C61-C62-C63	-2.9(4)	C2S-C3S-C4S-C5S	-2.3(13)
B-C61-C62-C63	-175.5(3)	C3S-C4S-C5S-C6S	0.6(17)
C61-C62-C63-C64	2.3(5)	C4S-C5S-C6S-C1S	1.4(18)
C61-C62-C63-C67	-177.7(3)	C2S-C1S-C6S-C5S	-2.0(16)
C62-C63-C64-C65	0.7(5)	F1S-C1S-C6S-C5S	177.5(10)
C67-C63-C64-C65	-179.3(4)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 23

Table S11. Crystal data and structure refinement for $[CpRu(N_2)(dippe)][BAr'_4]$ - **2a**.

Identification code	pvj_575
Empirical formula	C51 H49 B F24 N2 P2 Ru
Formula weight	1319.74
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2(1)/n (no. 14)
Unit cell dimensions	a = 12.391(4) Å α = 90 deg.
	b = 35.677(12) Å β = 90.01(1) deg.
	c = 12.885(4) Å γ = 90 deg.
Volume	5696(3) $Å^3$
Z, Calculated density	4, 1.539 Mg/m^3
Absorption coefficient	0.447 mm^{-1}
F(000)	2656
Crystal size	0.46 x 0.42 x 0.38 mm, yellow block
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 15 sec. per frame full sphere data collection, 4 x 606 frames
Theta range for data collection	1.74 to 30.00 deg.
Index ranges	-17 <= h <= 17, -50 <= k <= 50, -17 <= l <= 17
Reflections collected / unique	82786 / 16486 [R(int)=0.0391, R(sigma)=0.0212]
Completeness to theta = 30.00	99.3%
Absorption correction	semi-empirical from equivalents (prg. SADABS)
Max. and min. transmission	0.894 and 0.756
Structure solution	direct methods (program SHELXS97)
Refinement method	full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	16486 / 0 / 773
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0639, wR2 = 0.1513 (13778 data)
R indices (all data)	R1 = 0.0754, wR2 = 0.1607 (16486 data)
Extinction coefficient	0.00127(16)
Largest diff. peak and hole	0.768 and -0.722 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S12. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[CpRu(N_2)(dippe)][BAr'_4]$ - **2a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	78086(2)	10140(1)	12360(2)	45(1)
P(1)	65180(7)	14853(2)	13676(6)	44(1)
P(2)	75767(7)	9686(2)	30230(6)	44(1)
N(1)	66260(30)	6566(8)	10250(20)	54(1)
N(2)	59980(30)	4532(10)	8530(30)	75(1)
C(1)	86370(50)	8560(20)	-2240(40)	97(2)
C(2)	91730(40)	6751(19)	6140(50)	99(2)
C(3)	95920(30)	9560(20)	12430(40)	90(2)
C(4)	93170(40)	13067(18)	8370(40)	86(2)
C(5)	87450(40)	12400(20)	-970(40)	93(2)
C(6)	57600(30)	13829(11)	25520(30)	56(1)
C(7)	65570(30)	13138(12)	34310(30)	62(1)
C(8)	54900(40)	15299(16)	3340(30)	77(1)
C(9)	59240(50)	14448(16)	-7350(30)	85(2)
C(10)	44300(50)	13940(30)	5400(50)	130(3)
C(11)	70390(30)	19662(11)	15890(40)	65(1)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 24

C(12)	75640(50)	21301(15)	6330(50)	101(2)
C(13)	61810(50)	22365(14)	20080(60)	108(2)
C(14)	69590(40)	5190(12)	34350(30)	67(1)
C(15)	75610(40)	1714(12)	30320(40)	78(1)
C(16)	67140(60)	4862(18)	45850(40)	107(2)
C(17)	86800(40)	10670(12)	39490(30)	64(1)
C(18)	92230(50)	14468(16)	37310(40)	92(2)
C(19)	95210(40)	7537(16)	40590(40)	84(1)
B	21220(20)	13311(8)	70630(20)	32(1)
C(21)	28080(20)	10133(7)	77090(20)	32(1)
C(22)	38350(20)	8899(8)	74120(20)	36(1)
C(23)	44170(20)	6333(8)	80000(20)	38(1)
C(24)	40090(20)	4900(9)	89150(20)	43(1)
C(25)	29990(30)	6100(10)	92350(20)	45(1)
C(26)	24180(20)	8654(9)	86490(20)	39(1)
C(27)	54980(30)	5023(11)	76300(30)	56(1)
C(28)	25200(40)	4605(15)	102150(30)	73(1)
C(31)	23810(20)	17171(8)	77050(20)	35(1)
C(32)	33530(20)	19119(8)	75760(20)	40(1)
C(33)	36410(20)	22083(9)	82070(30)	46(1)
C(34)	29770(30)	23255(10)	90070(30)	53(1)
C(35)	20150(30)	21377(10)	91490(30)	52(1)
C(36)	17280(20)	18389(9)	85220(20)	42(1)
C(37)	46900(30)	24142(11)	80340(30)	60(1)
C(38)	12900(40)	22537(16)	100260(40)	86(2)
C(41)	8360(20)	12252(7)	70452(19)	32(1)
C(42)	350(20)	14968(8)	68860(20)	38(1)
C(43)	-10500(20)	14031(9)	68070(20)	41(1)
C(44)	-13870(20)	10334(9)	68730(20)	41(1)
C(45)	-6070(20)	7599(8)	70100(20)	38(1)
C(46)	4760(20)	8556(8)	70930(20)	35(1)
C(47)	-18650(30)	17091(12)	66610(30)	59(1)
C(48)	-9140(30)	3533(10)	70710(30)	50(1)
C(51)	24680(20)	13414(8)	58380(20)	36(1)
C(52)	25590(20)	16661(9)	52420(20)	42(1)
C(53)	27820(30)	16526(10)	41770(20)	47(1)
C(54)	29240(30)	13162(10)	36740(20)	51(1)
C(55)	28320(30)	9899(9)	42460(30)	50(1)
C(56)	26090(30)	10013(9)	52990(20)	44(1)
C(57)	29170(40)	20113(12)	35800(30)	71(1)
C(58)	30000(50)	6216(12)	37000(30)	79(1)
F(27A) §	59738(19)	7430(9)	70090(20)	96(1)
F(27F)	62937(19)	7372(9)	78870(30)	148(2)
F(27B)	61970(20)	4586(11)	83980(20)	119(2)
F(27D)	57810(30)	1859(9)	80310(30)	96(1)
F(27C)	54610(30)	1917(9)	71540(30)	148(2)
F(27E)	55570(20)	4703(11)	66430(20)	119(2)
F(28A)	31980(30)	2897(11)	108120(20)	129(2)
F(28F)	29340(30)	6031(11)	110540(20)	163(2)
F(28B)	20690(30)	7245(11)	107840(20)	118(2)
F(28D)	14700(30)	5325(13)	102730(30)	129(2)
F(28C)	17340(40)	2192(12)	100320(30)	163(2)
F(28E)	25980(40)	978(9)	103010(30)	118(2)
F(37A)	51100(20)	25351(11)	89180(20)	130(2)
F(37F)	46460(20)	27617(8)	83840(30)	102(1)
F(37B)	45750(20)	27126(8)	74600(30)	104(1)
F(37D)	49680(20)	24370(9)	70690(20)	130(2)
F(37C)	54325(19)	22104(8)	76030(30)	102(1)
F(37E)	55040(20)	22595(9)	85280(30)	104(1)
F(38A)	15200(40)	20910(30)	108580(30)	243(6)
F(38F)	18040(30)	24030(30)	107650(50)	101(2)
F(38B)	13220(50)	26075(15)	102270(60)	199(5)
F(38D)	5570(40)	25012(11)	97820(40)	243(6)
F(38C)	2730(30)	21899(12)	98760(30)	101(2)
F(38E)	7550(40)	19849(14)	104130(40)	199(5)
F(47A)	-27930(30)	15914(10)	63180(40)	138(2)
F(47F)	-22050(30)	17464(12)	57230(30)	111(2)
F(47B)	-15600(30)	19680(10)	60330(30)	128(2)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 25

F(47D)	-15020(30)	20346(8)	69390(30)	138(2)
F(47C)	-20900(30)	18795(10)	75350(30)	111(2)
F(47E)	-27350(20)	16579(10)	72240(30)	128(2)
F(48A)	-19378(18)	2949(7)	71180(30)	108(2)
F(48F)	-14920(20)	2400(7)	62970(20)	105(1)
F(48B)	-5450(20)	1577(7)	62770(20)	84(1)
F(48D)	-440(20)	1303(7)	70800(30)	108(2)
F(48C)	-4900(30)	1851(8)	79010(20)	105(1)
F(48E)	-14370(30)	2674(8)	79200(20)	84(1)
F(57A)	32160(70)	19640(20)	26190(40)	92(3)
F(57B)	38180(60)	22140(18)	39820(50)	101(3)
F(57C)	21570(60)	22400(20)	36430(70)	109(4)
F(57D)	25800(130)	22890(30)	40240(90)	124(6)
F(57E)	20330(150)	19930(40)	27870(90)	162(7)
F(57F)	36430(110)	20420(40)	30420(140)	184(12)
F(58A)	29920(80)	3317(13)	43060(30)	123(4)
F(58B)	21220(50)	5592(17)	30230(40)	100(2)
F(58C)	38340(50)	6188(19)	31000(60)	113(3)
F(58D)	34000(300)	6430(80)	28530(130)	184(18)
F(58E)	39800(200)	4570(60)	42470(180)	147(10)
F(58F)	23760(150)	4010(50)	39000(300)	174(16)

Remarks: §) The CF_3 groups showed significant orientation disorder and were refined with fluorine positions splitted into two sets of each three F positions. For this purpose the fluorine atoms were restrained to form idealized hexagons with anisotropic temperature factors of opposite F atoms restrained to be equal. For $C(57)F_3$ and $C(58)F_3$ the F atoms were restrained to form two independent equilateral triangles but U_{ij} were not restrained. Refined site occupation factors for the predominately (A,B,C)/subordinately (D,E,F) sets of sites F sites were: F(27#) 0.908(6)/0.092(6), F(28#) 0.918(6)/0.082(6), F(37#) 0.926(5)/0.074(6), F(38#) 0.771(6)/0.229(6), F(47#) 0.853(6)/0.147(6), F(48#) 0.923(5)/0.077(5), F(57#) 0.585(11)/0.415(11), and F(58#) 0.744(13)/0.256(13).

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[CpRu(N_2)(dippe)][BAr'_4]$ - **2a**.

	x	y	z	U_{eq}
H(1)	8299	729	-825	117
H(2)	9280	402	701	119
H(3)	10040	914	1869	108
H(4)	9554	1553	1104	103
H(5)	8493	1435	-590	111
H(6A)	5289	1595	2725	67
H(6B)	5308	1161	2449	67
H(7A)	6172	1220	4043	74
H(7B)	6913	1550	3620	74
H(8)	5376	1804	303	93
H(9A)	5350	1472	-1242	128
H(9B)	6198	1190	-752	128
H(9C)	6503	1618	-898	128
H(10A)	3978	1433	-64	195
H(10B)	4129	1527	1129	195
H(10C)	4463	1128	696	195
H(11)	7607	1947	2126	78
H(12A)	7823	2381	786	152
H(12B)	7040	2142	74	152
H(12C)	8165	1973	424	152
H(13A)	6499	2482	2108	161
H(13B)	5909	2144	2665	161
H(13C)	5591	2254	1515	161
H(14)	6246	512	3088	80
H(15A)	7195	-53	3269	116
H(15B)	8295	173	3294	116
H(15C)	7573	175	2279	116
H(16A)	6387	244	4725	160

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 26

H(16B)	6220	684	4788	160
H(16C)	7378	509	4978	160
H(17)	8334	1091	4638	76
H(18A)	9792	1489	4235	137
H(18B)	8691	1645	3783	137
H(18C)	9529	1445	3038	137
H(19A)	10066	828	4558	126
H(19B)	9860	709	3392	126
H(19C)	9170	526	4295	126
H(22)	4141	984	6797	43
H(24)	4406	316	9309	52
H(26)	1738	943	8889	47
H(32)	3825	1839	7042	47
H(34)	3174	2526	9439	64
H(36)	1074	1714	8650	50
H(42)	239	1750	6831	46
H(44)	-2122	970	6827	50
H(46)	986	663	7186	42
H(52)	2468	1900	5564	50
H(54)	3078	1308	2960	61
H(56)	2549	775	5667	52

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S14. Anisotropic displacement parameters ($Å^2$ x 10^3) for [CpRu(N_2)(dippe)][BAr'$_4$] - **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	43(1)	57(1)	35(1)	-3(1)	5(1)	1(1)
P(1)	45(1)	44(1)	43(1)	3(1)	-1(1)	-4(1)
P(2)	49(1)	50(1)	34(1)	1(1)	1(1)	2(1)
N(1)	63(2)	48(2)	50(2)	-5(1)	-11(1)	1(1)
N(2)	86(3)	55(2)	85(3)	-3(2)	-31(2)	-8(2)
C(1)	84(3)	155(6)	52(3)	-22(3)	22(2)	8(4)
C(2)	75(3)	111(4)	111(5)	-17(4)	34(3)	30(3)
C(3)	43(2)	152(6)	74(3)	2(3)	15(2)	12(3)
C(4)	56(2)	122(4)	78(3)	5(3)	26(2)	-16(3)
C(5)	70(3)	148(6)	60(3)	27(3)	28(2)	6(3)
C(6)	50(2)	59(2)	59(2)	3(2)	12(2)	9(2)
C(7)	76(2)	67(2)	43(2)	-5(2)	14(2)	13(2)
C(8)	62(2)	105(4)	64(2)	12(2)	-19(2)	6(2)
C(9)	106(4)	95(4)	55(2)	0(2)	-29(2)	0(3)
C(10)	75(4)	211(9)	102(5)	-19(5)	-22(3)	-28(4)
C(11)	66(2)	50(2)	79(3)	-1(2)	-10(2)	-7(2)
C(12)	122(5)	66(3)	116(4)	24(3)	5(4)	-31(3)
C(13)	108(4)	50(2)	164(6)	-31(3)	-5(4)	-1(3)
C(14)	75(3)	63(2)	62(2)	15(2)	1(2)	-9(2)
C(15)	95(3)	54(2)	83(3)	10(2)	-17(3)	-5(2)
C(16)	143(6)	103(4)	74(3)	36(3)	18(3)	-15(4)
C(17)	77(3)	69(2)	45(2)	-3(2)	-15(2)	-3(2)
C(18)	100(4)	94(4)	80(3)	-11(3)	-28(3)	-29(3)
C(19)	75(3)	106(4)	72(3)	3(3)	-28(2)	9(3)
B	29(1)	34(1)	33(1)	2(1)	1(1)	2(1)
C(21)	29(1)	35(1)	32(1)	-1(1)	-1(1)	1(1)
C(22)	30(1)	37(1)	40(1)	-2(1)	2(1)	0(1)
C(23)	28(1)	41(1)	45(2)	-6(1)	-3(1)	3(1)
C(24)	42(2)	44(2)	44(2)	0(1)	-10(1)	9(1)
C(25)	43(2)	59(2)	34(1)	6(1)	-2(1)	7(1)
C(26)	33(1)	51(2)	33(1)	2(1)	3(1)	8(1)
C(27)	40(2)	60(2)	66(2)	2(2)	6(2)	15(2)
C(28)	73(3)	98(3)	48(2)	28(2)	8(2)	23(2)
C(31)	33(1)	36(1)	37(1)	1(1)	1(1)	0(1)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 27

C(32)	33(1)	38(1)	47(2)	0(1)	4(1)	-1(1)
C(33)	34(1)	42(2)	61(2)	-2(1)	0(1)	-7(1)
C(34)	46(2)	52(2)	61(2)	-18(2)	2(2)	-9(1)
C(35)	47(2)	58(2)	50(2)	-18(2)	11(1)	-8(1)
C(36)	37(1)	47(2)	42(1)	-6(1)	6(1)	-7(1)
C(37)	41(2)	53(2)	85(3)	-6(2)	4(2)	-11(2)
C(38)	66(3)	114(4)	77(3)	-54(3)	21(2)	-23(3)
C(41)	31(1)	37(1)	29(1)	1(1)	2(1)	3(1)
C(42)	37(1)	41(1)	37(1)	2(1)	-1(1)	7(1)
C(43)	35(1)	49(2)	37(1)	1(1)	-2(1)	12(1)
C(44)	28(1)	56(2)	40(1)	-4(1)	-1(1)	2(1)
C(45)	32(1)	45(2)	37(1)	-5(1)	1(1)	-3(1)
C(46)	30(1)	37(1)	38(1)	-1(1)	-1(1)	4(1)
C(47)	44(2)	67(2)	66(2)	5(2)	-3(2)	20(2)
C(48)	39(2)	48(2)	62(2)	-6(2)	4(1)	-6(1)
C(51)	32(1)	40(1)	35(1)	1(1)	0(1)	2(1)
C(52)	43(2)	42(2)	40(1)	4(1)	4(1)	9(1)
C(53)	49(2)	52(2)	41(2)	11(1)	5(1)	11(1)
C(54)	59(2)	59(2)	35(1)	1(1)	4(1)	4(2)
C(55)	63(2)	47(2)	40(2)	-7(1)	1(1)	-1(2)
C(56)	52(2)	41(2)	38(1)	-2(1)	1(1)	-5(1)
C(57)	102(3)	58(2)	53(2)	18(2)	21(2)	29(2)
C(58)	129(4)	54(2)	52(2)	-15(2)	18(3)	-12(3)
F(27A)	42(1)	118(3)	128(3)	45(2)	33(2)	22(2)
F(27F)	91(3)	102(3)	250(6)	-95(3)	66(3)	6(2)
F(27B)	54(2)	210(5)	93(2)	18(3)	-4(2)	65(2)
F(27D)	42(1)	118(3)	128(3)	45(2)	33(2)	22(2)
F(27C)	91(3)	102(3)	250(6)	-95(3)	66(3)	6(2)
F(27E)	54(2)	210(5)	93(2)	18(3)	-4(2)	65(2)
F(28A)	124(3)	197(4)	65(2)	71(2)	27(2)	86(3)
F(28F)	198(5)	197(5)	95(3)	43(3)	28(3)	-112(4)
F(28B)	124(3)	173(4)	57(2)	35(2)	44(2)	69(3)
F(28D)	124(3)	197(4)	65(2)	71(2)	27(2)	86(3)
F(28C)	198(5)	197(5)	95(3)	43(3)	28(3)	-112(4)
F(28E)	124(3)	173(4)	57(2)	35(2)	44(2)	69(3)
F(37A)	77(2)	199(5)	115(3)	-34(3)	-4(2)	-77(3)
F(37F)	44(1)	73(2)	189(4)	-19(2)	38(2)	-10(1)
F(37B)	67(2)	68(2)	176(4)	34(2)	17(2)	-16(1)
F(37D)	77(2)	199(5)	115(3)	-34(3)	-4(2)	-77(3)
F(37C)	44(1)	73(2)	189(4)	-19(2)	38(2)	-10(1)
F(37E)	67(2)	68(2)	176(4)	34(2)	17(2)	-16(1)
F(38A)	176(6)	506(17)	46(2)	16(5)	33(3)	150(9)
F(38F)	68(2)	113(3)	123(3)	-55(3)	49(2)	-15(2)
F(38B)	166(5)	127(4)	303(9)	-154(6)	161(6)	-76(4)
F(38D)	176(6)	506(17)	46(2)	16(5)	33(3)	150(9)
F(38C)	68(2)	113(3)	123(3)	-55(3)	49(2)	-15(2)
F(38E)	166(5)	127(4)	303(9)	-154(6)	161(6)	-76(4)
F(47A)	63(2)	100(3)	253(6)	-14(3)	-75(3)	33(2)
F(47F)	122(3)	109(3)	101(3)	-12(2)	12(2)	76(2)
F(47B)	89(3)	131(3)	164(4)	100(3)	39(3)	64(2)
F(47D)	63(2)	100(3)	253(6)	-14(3)	-75(3)	33(2)
F(47C)	122(3)	109(3)	101(3)	-12(2)	12(2)	76(2)
F(47E)	89(3)	131(3)	164(4)	100(3)	39(3)	64(2)
F(48A)	40(1)	57(2)	228(5)	-27(2)	27(2)	-15(1)
F(48F)	152(3)	63(2)	100(2)	32(2)	-34(2)	-38(2)
F(48B)	98(2)	51(1)	104(2)	-23(1)	35(2)	-4(1)
F(48D)	40(1)	57(2)	228(5)	-27(2)	27(2)	-15(1)
F(48C)	152(3)	63(2)	100(2)	32(2)	-34(2)	-38(2)
F(48E)	98(2)	51(1)	104(2)	-23(1)	35(2)	-4(1)
F(57A)	165(10)	68(3)	42(2)	16(2)	26(3)	29(4)
F(57B)	122(6)	85(4)	95(4)	36(3)	-15(4)	-47(4)
F(57C)	87(4)	100(6)	139(9)	62(6)	45(5)	66(4)
F(57D)	232(19)	57(5)	82(6)	36(4)	28(9)	25(8)
F(57E)	238(18)	159(11)	90(7)	55(7)	-57(9)	41(10)
F(57F)	129(12)	147(15)	280(20)	150(17)	141(16)	75(11)
F(58A)	266(11)	42(2)	62(2)	-6(2)	2(4)	15(4)
F(58B)	129(4)	98(4)	74(3)	-38(2)	-10(3)	-33(3)
F(58C)	111(4)	74(3)	153(8)	-50(4)	55(4)	-2(3)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 28

F(58D)	380(50)	132(17)	35(7)	-34(8)	33(15)	20(30)
F(58E)	190(20)	87(11)	170(20)	-81(12)	-27(15)	56(12)
F(58F)	133(15)	64(12)	330(50)	-79(19)	-30(20)	-28(11)

For F atoms see remarks in Table 12.

Table S15. Bond lengths [Å] and angles [deg] for $[CpRu(N_2)(dippe)][BAr'_4]$ - **2a**.

Bond distances

Ru-N(1)	1.961(3)
Ru-C(4)	2.202(4)
Ru-C(1)	2.216(4)
Ru-C(3)	2.220(4)
Ru-C(5)	2.224(4)
Ru-C(2)	2.228(5)
Ru-P(2)	2.326(1)
Ru-P(1)	2.327(1)
P(1)-C(6)	1.830(4)
P(1)-C(8)	1.849(4)
P(1)-C(11)	1.855(4)
P(2)-C(7)	1.841(4)
P(2)-C(17)	1.848(4)
P(2)-C(14)	1.855(4)
N(1)-N(2)	1.087(4)
C(1)-C(5)	1.389(9)
C(1)-C(2)	1.422(8)
C(1)-H(1)	0.99
C(2)-C(3)	1.390(8)
C(2)-H(2)	0.99
C(3)-C(4)	1.399(8)
C(3)-H(3)	0.99
C(4)-C(5)	1.416(8)
C(4)-H(4)	0.99
C(5)-H(5)	0.99
C(6)-C(7)	1.523(5)
C(6)-H(6A)	0.98
C(6)-H(6B)	0.98
C(7)-H(7A)	0.98
C(7)-H(7B)	0.98
C(8)-C(10)	1.425(7)
C(8)-C(9)	1.510(7)
C(8)-H(8)	0.99
C(9)-H(9A)	0.97
C(9)-H(9B)	0.97
C(9)-H(9C)	0.97
C(10)-H(10A)	0.97
C(10)-H(10B)	0.97
C(10)-H(10C)	0.97
C(11)-C(12)	1.511(7)
C(11)-C(13)	1.534(7)
C(11)-H(11)	0.99
C(12)-H(12A)	0.97
C(12)-H(12B)	0.97
C(12)-H(12C)	0.97
C(13)-H(13A)	0.97
C(13)-H(13B)	0.97
C(13)-H(13C)	0.97
C(14)-C(16)	1.517(7)
C(14)-C(15)	1.538(6)
C(14)-H(14)	0.99
C(15)-H(15A)	0.97
C(15)-H(15B)	0.97
C(15)-H(15C)	0.97
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
C(16)-H(16C)	0.97
C(17)-C(19)	1.535(6)
C(17)-C(18)	1.539(7)
C(17)-H(17)	0.99
C(18)-H(18A)	0.97
C(18)-H(18B)	0.97
C(18)-H(18C)	0.97
C(19)-H(19A)	0.97
C(19)-H(19B)	0.97
C(19)-H(19C)	0.97
B-C(51)	1.635(4)
B-C(41)	1.637(4)
B-C(31)	1.639(4)
B-C(21)	1.644(4)
C(21)-C(22)	1.401(4)
C(21)-C(26)	1.407(4)
C(22)-C(23)	1.389(4)
C(22)-H(22)	0.94
C(23)-C(24)	1.381(4)
C(23)-C(27)	1.497(4)
C(24)-C(25)	1.386(4)
C(24)-H(24)	0.94
C(25)-C(26)	1.385(4)
C(25)-C(28)	1.494(5)
C(26)-H(26)	0.94
C(27)-F(27C)	1.268(5)
C(27)-F(27E)	1.279(5)
C(27)-F(27D)	1.290(4)
C(27)-F(27A)	1.313(5)
C(27)-F(27B)	1.324(5)
C(27)-F(27F)	1.335(5)
C(28)-F(28A)	1.292(5)
C(28)-F(28F)	1.299(6)
C(28)-F(28E)	1.303(6)
C(28)-F(28B)	1.317(6)
C(28)-F(28C)	1.320(6)
C(28)-F(28D)	1.328(5)
C(31)-C(36)	1.397(4)
C(31)-C(32)	1.400(4)
C(32)-C(33)	1.381(4)
C(32)-H(32)	0.94
C(33)-C(34)	1.384(5)
C(33)-C(37)	1.509(4)
C(34)-C(35)	1.380(5)
C(34)-H(34)	0.94
C(35)-C(36)	1.383(4)
C(35)-C(38)	1.502(5)
C(36)-H(36)	0.94
C(37)-F(37D)	1.293(5)
C(37)-F(37C)	1.297(5)
C(37)-F(37B)	1.304(5)
C(37)-F(37E)	1.314(5)
C(37)-F(37F)	1.320(5)
C(37)-F(37A)	1.325(5)
C(38)-F(38A)	1.252(8)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 29

C(38)-F(38F)	1.262(5)
C(38)-F(38E)	1.268(7)
C(38)-F(38B)	1.289(7)
C(38)-F(38C)	1.295(5)
C(38)-F(38D)	1.305(7)
C(41)-C(46)	1.393(4)
C(41)-C(42)	1.402(4)
C(42)-C(43)	1.389(4)
C(42)-H(42)	0.94
C(43)-C(44)	1.386(4)
C(43)-C(47)	1.499(4)
C(44)-C(45)	1.384(4)
C(44)-H(44)	0.94
C(45)-C(46)	1.389(4)
C(45)-C(48)	1.502(4)
C(46)-H(46)	0.94
C(47)-F(47B)	1.284(5)
C(47)-F(47F)	1.287(5)
C(47)-F(47D)	1.296(5)
C(47)-F(47A)	1.302(5)
C(47)-F(47C)	1.310(5)
C(47)-F(47E)	1.313(5)
C(48)-F(48A)	1.287(4)
C(48)-F(48F)	1.293(4)
C(48)-F(48E)	1.308(4)
C(48)-F(48B)	1.320(4)
C(48)-F(48C)	1.335(4)
C(48)-F(48D)	1.341(4)
C(51)-C(52)	1.395(4)
C(51)-C(56)	1.409(4)
C(52)-C(53)	1.400(4)
C(52)-H(52)	0.94
C(53)-C(54)	1.376(5)
C(53)-C(57)	1.503(5)
C(54)-C(55)	1.383(5)
C(54)-H(54)	0.94
C(55)-C(56)	1.386(4)
C(55)-C(58)	1.505(5)
C(56)-H(56)	0.94
C(57)-F(57F)	1.141(10)
C(57)-F(57D)	1.220(13)
C(57)-F(57C)	1.249(7)
C(57)-F(57A)	1.303(7)
C(57)-F(57B)	1.428(7)
C(57)-F(57E)	1.499(12)
C(58)-F(58F)	1.13(2)
C(58)-F(58D)	1.20(2)
C(58)-F(58C)	1.291(8)
C(58)-F(58A)	1.296(6)
C(58)-F(58B)	1.412(8)
C(58)-F(58E)	1.52(2)

Bond angles

N(1)-Ru-C(4)	155.51(18)
N(1)-Ru-C(1)	93.6(2)
C(4)-Ru-C(1)	61.9(2)
N(1)-Ru-C(3)	133.1(2)
C(4)-Ru-C(3)	36.9(2)
C(1)-Ru-C(3)	61.2(2)
N(1)-Ru-C(5)	121.2(2)
C(4)-Ru-C(5)	37.3(2)
C(1)-Ru-C(5)	36.4(2)
C(3)-Ru-C(5)	61.2(2)
N(1)-Ru-C(2)	99.4(2)
C(4)-Ru-C(2)	61.9(2)
C(1)-Ru-C(2)	37.3(2)
C(3)-Ru-C(2)	36.4(2)
C(5)-Ru-C(2)	61.5(2)
N(1)-Ru-P(2)	89.98(9)
C(4)-Ru-P(2)	111.67(15)
C(1)-Ru-P(2)	151.61(18)
C(3)-Ru-P(2)	96.45(14)
C(5)-Ru-P(2)	148.65(17)
C(2)-Ru-P(2)	114.34(18)
N(1)-Ru-P(1)	88.09(10)
C(4)-Ru-P(1)	104.93(17)
C(1)-Ru-P(1)	124.37(19)
C(3)-Ru-P(1)	138.71(19)
C(5)-Ru-P(1)	98.76(17)
C(2)-Ru-P(1)	160.07(18)
P(2)-Ru-P(1)	83.86(3)
C(6)-P(1)-C(8)	105.3(2)
C(6)-P(1)-C(11)	103.6(2)
C(8)-P(1)-C(11)	105.7(2)
C(6)-P(1)-Ru	105.64(12)
C(8)-P(1)-Ru	118.88(18)
C(11)-P(1)-Ru	116.13(14)
C(7)-P(2)-C(17)	101.3(2)
C(7)-P(2)-C(14)	102.3(2)
C(17)-P(2)-C(14)	106.5(2)
C(7)-P(2)-Ru	108.74(12)
C(17)-P(2)-Ru	122.31(15)
C(14)-P(2)-Ru	113.25(14)
N(2)-N(1)-Ru	175.8(4)
C(5)-C(1)-C(2)	108.3(5)
C(5)-C(1)-Ru	72.1(3)
C(2)-C(1)-Ru	71.8(3)
C(5)-C(1)-H(1)	125.8
C(2)-C(1)-H(1)	125.8
Ru-C(1)-H(1)	125.8
C(3)-C(2)-C(1)	106.9(6)
C(3)-C(2)-Ru	71.4(3)
C(1)-C(2)-Ru	70.9(3)
C(3)-C(2)-H(2)	126.5
C(1)-C(2)-H(2)	126.5
Ru-C(2)-H(2)	126.5
C(2)-C(3)-C(4)	109.6(5)
C(2)-C(3)-Ru	72.1(3)
C(4)-C(3)-Ru	70.9(3)
C(2)-C(3)-H(3)	125.2
C(4)-C(3)-H(3)	125.2
Ru-C(3)-H(3)	125.2
C(3)-C(4)-C(5)	106.9(6)
C(3)-C(4)-Ru	72.3(3)
C(5)-C(4)-Ru	72.2(3)
C(3)-C(4)-H(4)	126.3
C(5)-C(4)-H(4)	126.3
Ru-C(4)-H(4)	126.3
C(1)-C(5)-C(4)	108.3(5)
C(1)-C(5)-Ru	71.5(3)
C(4)-C(5)-Ru	70.5(2)
C(1)-C(5)-H(5)	125.8
C(4)-C(5)-H(5)	125.8
Ru-C(5)-H(5)	125.8
C(7)-C(6)-P(1)	108.6(3)
C(7)-C(6)-H(6A)	110.0
P(1)-C(6)-H(6A)	110.0
C(7)-C(6)-H(6B)	110.0
P(1)-C(6)-H(6B)	110.0
H(6A)-C(6)-H(6B)	108.3
C(6)-C(7)-P(2)	109.9(2)
C(6)-C(7)-H(7A)	109.7
P(2)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7B)	109.7

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 30

P(2)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(10)-C(8)-C(9)	115.4(5)
C(10)-C(8)-P(1)	118.1(4)
C(9)-C(8)-P(1)	113.2(3)
C(10)-C(8)-H(8)	102.3
C(9)-C(8)-H(8)	102.3
P(1)-C(8)-H(8)	102.3
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(13)	110.0(4)
C(12)-C(11)-P(1)	112.5(3)
C(13)-C(11)-P(1)	113.2(3)
C(12)-C(11)-H(11)	106.9
C(13)-C(11)-H(11)	106.9
P(1)-C(11)-H(11)	106.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(16)-C(14)-C(15)	111.4(4)
C(16)-C(14)-P(2)	115.4(4)
C(15)-C(14)-P(2)	113.6(3)
C(16)-C(14)-H(14)	105.1
C(15)-C(14)-H(14)	105.1
P(2)-C(14)-H(14)	105.1
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(19)-C(17)-C(18)	111.1(4)
C(19)-C(17)-P(2)	115.0(3)
C(18)-C(17)-P(2)	111.9(3)
C(19)-C(17)-H(17)	106.0
C(18)-C(17)-H(17)	106.0
P(2)-C(17)-H(17)	106.0
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(51)-B-C(41)	104.3(2)
C(51)-B-C(31)	114.6(2)
C(41)-B-C(31)	113.1(2)
C(51)-B-C(21)	111.6(2)
C(41)-B-C(21)	110.6(2)
C(31)-B-C(21)	102.8(2)
C(22)-C(21)-C(26)	115.4(2)
C(22)-C(21)-B	123.3(2)
C(26)-C(21)-B	121.2(2)
C(23)-C(22)-C(21)	122.0(3)
C(23)-C(22)-H(22)	119.0
C(21)-C(22)-H(22)	119.0
C(24)-C(23)-C(22)	121.3(3)
C(24)-C(23)-C(27)	118.9(3)
C(22)-C(23)-C(27)	119.8(3)
C(23)-C(24)-C(25)	118.0(3)
C(23)-C(24)-H(24)	121.0
C(25)-C(24)-H(24)	121.0
C(26)-C(25)-C(24)	120.7(3)
C(26)-C(25)-C(28)	119.3(3)
C(24)-C(25)-C(28)	120.0(3)
C(25)-C(26)-C(21)	122.5(3)
C(25)-C(26)-H(26)	118.7
C(21)-C(26)-H(26)	118.7
F(27A)-C(27)-C(23)	113.1(3)
F(27B)-C(27)-C(23)	112.6(3)
F(27C)-C(27)-C(23)	113.2(3)
F(27C)-C(27)-F(27A)	107.0(3)
F(27C)-C(27)-F(27B)	106.4(3)
F(27A)-C(27)-F(27B)	103.8(3)
F(28A)-C(28)-C(25)	114.4(4)
F(28B)-C(28)-C(25)	112.6(4)
F(28C)-C(28)-C(25)	112.0(4)
F(28A)-C(28)-F(28B)	106.4(4)
F(28A)-C(28)-F(28C)	106.2(4)
F(28B)-C(28)-F(28C)	104.7(3)
C(36)-C(31)-C(32)	115.7(3)
C(36)-C(31)-B	121.9(2)
C(32)-C(31)-B	121.7(2)
C(33)-C(32)-C(31)	122.1(3)
C(33)-C(32)-H(32)	118.9
C(31)-C(32)-H(32)	118.9
C(32)-C(33)-C(34)	121.1(3)
C(32)-C(33)-C(37)	120.5(3)
C(34)-C(33)-C(37)	118.4(3)
C(35)-C(34)-C(33)	117.8(3)
C(35)-C(34)-H(34)	121.1
C(33)-C(34)-H(34)	121.1
C(34)-C(35)-C(36)	121.2(3)
C(34)-C(35)-C(38)	118.9(3)
C(36)-C(35)-C(38)	119.9(3)
C(35)-C(36)-C(31)	122.1(3)
C(35)-C(36)-H(36)	119.0
C(31)-C(36)-H(36)	119.0
F(37A)-C(37)-C(33)	111.7(3)
F(37B)-C(37)-C(33)	112.8(3)
F(37C)-C(37)-C(33)	113.6(3)
F(37C)-C(37)-F(37B)	107.0(3)
F(37C)-C(37)-F(37A)	105.8(3)
F(37B)-C(37)-F(37A)	105.4(3)
F(38A)-C(38)-C(35)	112.4(5)
F(38B)-C(38)-C(35)	113.8(5)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 31

F(38C)-C(38)-C(35)	114.9(4)
F(38A)-C(38)-F(38B)	105.9(3)
F(38A)-C(38)-F(38C)	105.6(4)
F(38B)-C(38)-F(38C)	103.4(5)
C(46)-C(41)-C(42)	115.7(2)
C(46)-C(41)-B	122.0(2)
C(42)-C(41)-B	122.1(2)
C(43)-C(42)-C(41)	122.0(3)
C(43)-C(42)-H(42)	119.0
C(41)-C(42)-H(42)	119.0
C(44)-C(43)-C(42)	121.1(3)
C(44)-C(43)-C(47)	119.9(3)
C(42)-C(43)-C(47)	119.1(3)
C(45)-C(44)-C(43)	117.9(3)
C(45)-C(44)-H(44)	121.0
C(43)-C(44)-H(44)	121.0
C(44)-C(45)-C(46)	120.7(3)
C(44)-C(45)-C(48)	120.7(3)
C(46)-C(45)-C(48)	118.6(3)
C(45)-C(46)-C(41)	122.6(3)
C(45)-C(46)-H(46)	118.7
C(41)-C(46)-H(46)	118.7
F(47A)-C(47)-C(43)	113.8(4)
F(47B)-C(47)-C(43)	113.9(3)
F(47C)-C(47)-C(43)	111.9(3)
F(47B)-C(47)-F(47A)	106.2(3)
F(47B)-C(47)-F(47C)	105.7(3)
F(47A)-C(47)-F(47C)	104.7(3)
F(48A)-C(48)-C(45)	114.1(3)
F(48B)-C(48)-C(45)	112.4(3)
F(48C)-C(48)-C(45)	112.1(3)
F(48A)-C(48)-F(48B)	107.0(3)
F(48A)-C(48)-F(48C)	106.2(3)
F(48B)-C(48)-F(48C)	104.3(3)
C(52)-C(51)-C(56)	115.7(3)
C(52)-C(51)-B	124.8(2)
C(56)-C(51)-B	119.2(2)
C(51)-C(52)-C(53)	121.8(3)
C(51)-C(52)-H(52)	119.1
C(53)-C(52)-H(52)	119.1
C(54)-C(53)-C(52)	121.2(3)
C(54)-C(53)-C(57)	119.1(3)
C(52)-C(53)-C(57)	119.7(3)
C(53)-C(54)-C(55)	118.2(3)
C(53)-C(54)-H(54)	120.9
C(55)-C(54)-H(54)	120.9
C(54)-C(55)-C(56)	121.0(3)
C(54)-C(55)-C(58)	118.3(3)
C(56)-C(55)-C(58)	120.7(3)
C(55)-C(56)-C(51)	122.2(3)
C(55)-C(56)-H(56)	118.9
C(51)-C(56)-H(56)	118.9
F(57A)-C(57)-C(53)	114.2(5)
F(57B)-C(57)-C(53)	109.4(4)
F(57C)-C(57)-C(53)	116.1(5)
F(57C)-C(57)-F(57A)	111.2(5)
F(57C)-C(57)-F(57B)	103.5(5)
F(57A)-C(57)-F(57B)	100.8(4)
F(58A)-C(58)-C(55)	114.5(4)
F(58B)-C(58)-C(55)	108.7(5)
F(58C)-C(58)-C(55)	113.4(5)
F(58C)-C(58)-F(58A)	111.2(5)
F(58C)-C(58)-F(58B)	104.2(4)
F(58A)-C(58)-F(58B)	103.9(5)

Torsion angles

N1-Ru-P1-C6	66.17(16)
C4-Ru-P1-C6	-134.9(2)
C1-Ru-P1-C6	159.2(3)
C3-Ru-P1-C6	-116.8(3)
C5-Ru-P1-C6	-172.5(2)
C2-Ru-P1-C6	179.1(6)
P2-Ru-P1-C6	-24.02(14)
N1-Ru-P1-C8	-51.7(2)
C4-Ru-P1-C8	107.3(2)
C1-Ru-P1-C8	41.3(3)
C3-Ru-P1-C8	125.3(3)
C5-Ru-P1-C8	69.6(3)
C2-Ru-P1-C8	61.2(6)
P2-Ru-P1-C8	-141.90(19)
N1-Ru-P1-C11	-179.67(18)
C4-Ru-P1-C11	-20.7(2)
C1-Ru-P1-C11	-86.6(3)
C3-Ru-P1-C11	-2.7(3)
C5-Ru-P1-C11	-58.3(2)
C2-Ru-P1-C11	-66.7(6)
P2-Ru-P1-C11	90.14(16)
N1-Ru-P2-C7	-87.71(18)
C4-Ru-P2-C7	104.0(2)
C1-Ru-P2-C7	174.7(4)
C3-Ru-P2-C7	138.8(2)
C5-Ru-P2-C7	97.1(4)
C2-Ru-P2-C7	171.9(3)
P1-Ru-P2-C7	0.36(16)
N1-Ru-P2-C17	154.95(19)
C4-Ru-P2-C17	-13.3(2)
C1-Ru-P2-C17	57.4(4)
C3-Ru-P2-C17	21.5(2)
C5-Ru-P2-C17	-20.2(4)
C2-Ru-P2-C17	54.6(3)
P1-Ru-P2-C17	-116.97(17)
N1-Ru-P2-C14	25.30(19)
C4-Ru-P2-C14	-143.0(2)
C1-Ru-P2-C14	-72.2(4)
C3-Ru-P2-C14	-108.2(2)
C5-Ru-P2-C14	-149.9(4)
C2-Ru-P2-C14	-75.1(3)
P1-Ru-P2-C14	113.37(17)
C4-Ru-N1-N2	-2(5)
C1-Ru-N1-N2	-3(4)
C3-Ru-N1-N2	-56(5)
C5-Ru-N1-N2	22(5)
C2-Ru-N1-N2	-40(4)
P2-Ru-N1-N2	-155(4)
P1-Ru-N1-N2	121(4)
N1-Ru-C1-C5	142.2(3)
C4-Ru-C1-C5	-37.3(3)
C3-Ru-C1-C5	-79.5(4)
C2-Ru-C1-C5	-117.0(5)
P2-Ru-C1-C5	-121.2(4)
P1-Ru-C1-C5	52.0(4)
N1-Ru-C1-C2	-100.9(4)
C4-Ru-C1-C2	79.6(4)
C3-Ru-C1-C2	37.4(4)
C5-Ru-C1-C2	117.0(5)
P2-Ru-C1-C2	-4.3(7)
P1-Ru-C1-C2	169.0(3)
C5-C1-C2-C3	0.5(6)
Ru-C1-C2-C3	-62.8(3)
C5-C1-C2-Ru	63.3(3)
N1-Ru-C2-C3	-160.4(4)
C4-Ru-C2-C3	36.5(3)
C1-Ru-C2-C3	116.1(6)
C5-Ru-C2-C3	79.1(4)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 32

P2-Ru-C2-C3	-66.1(4)
P1-Ru-C2-C3	88.5(7)
N1-Ru-C2-C1	83.5(4)
C4-Ru-C2-C1	-79.6(4)
C3-Ru-C2-C1	-116.1(6)
C5-Ru-C2-C1	-37.0(4)
P2-Ru-C2-C1	177.8(4)
P1-Ru-C2-C1	-27.6(8)
C1-C2-C3-C4	1.1(5)
Ru-C2-C3-C4	-61.3(3)
C1-C2-C3-Ru	62.4(3)
N1-Ru-C3-C2	27.0(5)
C4-Ru-C3-C2	-119.0(5)
C1-Ru-C3-C2	-38.4(4)
C5-Ru-C3-C2	-80.2(4)
P2-Ru-C3-C2	123.1(4)
P1-Ru-C3-C2	-148.9(3)
N1-Ru-C3-C4	146.0(3)
C1-Ru-C3-C4	80.6(4)
C5-Ru-C3-C4	38.8(3)
C2-Ru-C3-C4	119.0(5)
P2-Ru-C3-C4	-117.9(3)
P1-Ru-C3-C4	-29.9(4)
C2-C3-C4-C5	-2.3(5)
Ru-C3-C4-C5	-64.4(3)
C2-C3-C4-Ru	62.1(3)
N1-Ru-C4-C3	-79.8(5)
C1-Ru-C4-C3	-78.6(4)
C5-Ru-C4-C3	-115.1(5)
C2-Ru-C4-C3	-36.0(3)
P2-Ru-C4-C3	70.9(3)
P1-Ru-C4-C3	160.1(3)
N1-Ru-C4-C5	35.3(7)
C1-Ru-C4-C5	36.5(4)
C3-Ru-C4-C5	115.1(5)
C2-Ru-C4-C5	79.0(4)
P2-Ru-C4-C5	-174.1(3)
P1-Ru-C4-C5	-84.8(4)
C2-C1-C5-C4	-1.9(5)
Ru-C1-C5-C4	61.2(3)
C2-C1-C5-Ru	-63.1(3)
C3-C4-C5-C1	2.6(5)
Ru-C4-C5-C1	-61.8(3)
C3-C4-C5-Ru	64.4(3)
N1-Ru-C5-C1	-45.7(4)
C4-Ru-C5-C1	118.0(5)
C3-Ru-C5-C1	79.6(4)
C2-Ru-C5-C1	37.9(4)
P2-Ru-C5-C1	128.6(4)
P1-Ru-C5-C1	-138.8(3)
N1-Ru-C5-C4	-163.7(3)
C1-Ru-C5-C4	-118.0(5)
C3-Ru-C5-C4	-38.4(4)
C2-Ru-C5-C4	-80.1(4)
P2-Ru-C5-C4	10.6(6)
P1-Ru-C5-C4	103.2(4)
C8-P1-C6-C7	176.0(3)
C11-P1-C6-C7	-73.2(3)
Ru-P1-C6-C7	49.3(3)
P1-C6-C7-P2	-50.5(3)
C17-P2-C7-C6	159.3(3)
C14-P2-C7-C6	-90.8(3)
Ru-P2-C7-C6	29.3(3)
C6-P1-C8-C10	-15.1(6)
C11-P1-C8-C10	-124.4(5)
Ru-P1-C8-C10	102.9(5)
C6-P1-C8-C9	-154.5(4)
C11-P1-C8-C9	96.2(4)
Ru-P1-C8-C9	-36.5(5)
C6-P1-C11-C12	-171.8(4)
C8-P1-C11-C12	-61.3(4)
Ru-P1-C11-C12	72.9(4)
C6-P1-C11-C13	-46.3(4)
C8-P1-C11-C13	64.2(4)
Ru-P1-C11-C13	-161.6(4)
C7-P2-C14-C16	-58.9(4)
C17-P2-C14-C16	47.0(5)
Ru-P2-C14-C16	-175.7(4)
C7-P2-C14-C15	170.7(3)
C17-P2-C14-C15	-83.4(4)
Ru-P2-C14-C15	53.9(4)
C7-P2-C17-C19	161.8(4)
C14-P2-C17-C19	55.2(4)
Ru-P2-C17-C19	-77.3(4)
C7-P2-C17-C18	-70.1(4)
C14-P2-C17-C18	-176.7(4)
Ru-P2-C17-C18	50.8(4)
C51-B-C21-C22	26.2(3)
C41-B-C21-C22	141.8(2)
C31-B-C21-C22	-97.2(3)
C51-B-C21-C26	-158.2(3)
C41-B-C21-C26	-42.5(3)
C31-B-C21-C26	78.4(3)
C26-C21-C22-C23	1.2(4)
B-C21-C22-C23	177.0(2)
C21-C22-C23-C24	-0.6(4)
C21-C22-C23-C27	178.2(3)
C22-C23-C24-C25	-0.1(5)
C27-C23-C24-C25	-178.9(3)
C23-C24-C25-C26	0.1(5)
C23-C24-C25-C28	179.5(4)
C24-C25-C26-C21	0.5(5)
C28-C25-C26-C21	-178.9(4)
C22-C21-C26-C25	-1.1(4)
B-C21-C26-C25	-177.1(3)
C24-C23-C27-F27C	81.8(4)
C22-C23-C27-F27C	-97.0(4)
C24-C23-C27-F27E	143.4(3)
C22-C23-C27-F27E	-35.4(5)
C24-C23-C27-F27D	20.6(5)
C22-C23-C27-F27D	-158.2(3)
C24-C23-C27-F27A	-156.2(3)
C22-C23-C27-F27A	24.9(5)
C24-C23-C27-F27B	-38.9(5)
C22-C23-C27-F27B	142.2(3)
C24-C23-C27-F27F	-97.4(4)
C22-C23-C27-F27F	83.7(4)
C26-C25-C28-F28A	-166.0(4)
C24-C25-C28-F28A	14.6(6)
C26-C25-C28-F28F	-104.7(4)
C24-C25-C28-F28F	76.0(5)
C26-C25-C28-F28E	132.9(4)
C24-C25-C28-F28E	-46.5(6)
C26-C25-C28-F28B	-44.5(6)
C24-C25-C28-F28B	136.2(4)
C26-C25-C28-F28C	73.2(5)
C24-C25-C28-F28C	-106.2(4)
C26-C25-C28-F28D	14.5(6)
C24-C25-C28-F28D	-164.9(4)
C51-B-C31-C36	147.6(3)
C41-B-C31-C36	28.2(4)
C21-B-C31-C36	-91.0(3)
C51-B-C31-C32	-42.4(3)
C41-B-C31-C32	-161.8(2)
C21-B-C31-C32	78.9(3)
C36-C31-C32-C33	-0.8(4)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 33

B-C31-C32-C33	-171.3(3)
C31-C32-C33-C34	0.3(5)
C31-C32-C33-C37	-179.2(3)
C32-C33-C34-C35	-0.3(5)
C37-C33-C34-C35	179.2(4)
C33-C34-C35-C36	0.8(6)
C33-C34-C35-C38	178.7(4)
C34-C35-C36-C31	-1.4(6)
C38-C35-C36-C31	-179.2(4)
C32-C31-C36-C35	1.3(5)
B-C31-C36-C35	171.8(3)
C32-C33-C37-F37C	-27.3(5)
C34-C33-C37-F37C	153.2(4)
C32-C33-C37-F37B	94.7(4)
C34-C33-C37-F37B	-84.8(5)
C32-C33-C37-F37A	-146.8(4)
C34-C33-C37-F37A	33.6(5)
C34-C35-C38-F38A	-87.0(7)
C36-C35-C38-F38A	90.8(6)
C34-C35-C38-F38B	33.3(8)
C36-C35-C38-F38B	-148.8(6)
C34-C35-C38-F38C	152.3(5)
C36-C35-C38-F38C	-29.9(7)
C51-B-C41-C46	91.2(3)
C31-B-C41-C46	-143.6(2)
C21-B-C41-C46	-28.9(3)
C51-B-C41-C42	-82.9(3)
C31-B-C41-C42	42.3(3)
C21-B-C41-C42	157.0(2)
C46-C41-C42-C43	1.5(4)
B-C41-C42-C43	175.9(2)
C41-C42-C43-C44	-0.6(4)
C41-C42-C43-C47	178.7(3)
C42-C43-C44-C45	-0.6(4)
C47-C43-C44-C45	-179.9(3)
C43-C44-C45-C46	1.0(4)
C43-C44-C45-C48	-179.1(3)
C44-C45-C46-C41	0.0(4)
C48-C45-C46-C41	180.0(3)
C42-C41-C46-C45	-1.2(4)
B-C41-C46-C45	-175.6(2)
C44-C43-C47-F47B	-140.3(4)
C42-C43-C47-F47B	40.4(5)
C44-C43-C47-F47A	-18.4(5)
C42-C43-C47-F47A	162.3(4)
C44-C43-C47-F47C	100.0(4)
C42-C43-C47-F47C	-79.4(4)
C44-C45-C48-F48A	-8.3(5)
C46-C45-C48-F48A	171.7(3)
C44-C45-C48-F48B	113.9(3)
C46-C45-C48-F48B	-66.2(4)
C44-C45-C48-F48C	-129.0(3)
C46-C45-C48-F48C	50.9(4)
C41-B-C51-C52	98.8(3)
C31-B-C51-C52	-25.4(4)
C21-B-C51-C52	-141.8(3)
C41-B-C51-C56	-75.9(3)
C31-B-C51-C56	159.9(3)
C21-B-C51-C56	43.5(3)
C56-C51-C52-C53	-0.3(4)
B-C51-C52-C53	-175.2(3)
C51-C52-C53-C54	-0.1(5)
C51-C52-C53-C57	-177.5(3)
C52-C53-C54-C55	0.4(5)
C57-C53-C54-C55	177.8(4)
C53-C54-C55-C56	-0.3(5)
C53-C54-C55-C58	-179.2(4)
C54-C55-C56-C51	-0.2(5)
C58-C55-C56-C51	178.7(4)
C52-C51-C56-C55	0.5(5)
B-C51-C56-C55	175.7(3)
C54-C53-C57-F57C	128.1(6)
C52-C53-C57-F57C	-54.5(8)
C54-C53-C57-F57A	-3.2(7)
C52-C53-C57-F57A	174.2(5)
C54-C53-C57-F57B	-115.3(5)
C52-C53-C57-F57B	62.1(6)
C54-C55-C58-F58C	45.4(7)
C56-C55-C58-F58C	-133.6(5)
C54-C55-C58-F58A	174.4(6)
C56-C55-C58-F58A	-4.6(8)
C54-C55-C58-F58B	-70.0(6)
C56-C55-C58-F58B	111.0(5)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 34

Table S16. Crystal data and structure refinement for $[CpRu(PMe^iPr_2)_3][BAr'_4]$ - **3**.

Identification code	pvej3fr
Empirical formula	C58 H68 B F24 P3 Ru
Formula weight	1425.91
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, Cc (No. 9)
	a = 21.264(9) Å α = 90 deg.
	b = 15.092(6) Å β = 106.06(1) deg.
	c = 20.992(9) Å γ = 90 deg.
Volume	6474(5) $Å^3$
Z, Calculated density	4, 1.463 Mg/m^3
Absorption coefficient	0.422 mm^{-1}
F(000)	2904
Crystal size	0.72 x 0.68 x 0.40 mm, yellow block
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 10 sec. per frame full sphere data collection, 4 x 606 frames
Theta range for data collection	1.68 to 27.50 deg.
Index ranges	-27 <= h <= 27, -19 <= k <= 19, -27 <= l <= 27
Reflections collected / unique	39811 / 14831 [R(int) = 0.0192]
Completeness to theta = 27.50	100.0%
Absorption correction	semi-empirical from equivalents (prg. SADABS)
Max. and min. transmission	0.86 and 0.80
Structure solution	direct methods (program SHELXS97)
Refinement method	full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	14831 / 50 / 886
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.1193 (12962 data)
R indices (all data)	R1 = 0.0561, wR2 = 0.1311 (14831 data)
Absolute structure parameter	0.84(2) (Polar space group, merohedral twin)
Extinction coefficient	0.00107(11)
Largest diff. peak and hole	0.473 and -0.856 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S17. Atomic coordinates ($x10^5$ for Ru, P; $x10^4$ for C,B,F) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $[CpRu(PMe^iPr_2)_3][BAr'_4]$ - **3**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	50000(1)	22111(2)	25000(1)	65(1)
P(1)	49515(6)	36889(11)	21105(7)	82(1)
P(2)	61396(5)	20664(7)	26861(5)	60(1)
P(3)	47332(6)	15501(10)	14369(6)	75(1)
C(1)	4676(4)	2524(5)	3406(3)	100(2)
C(2)	5089(4)	1768(6)	3540(3)	109(2)
C(3)	4737(5)	1121(5)	3090(4)	117(3)
C(4)	4166(4)	1442(8)	2689(4)	127(3)
C(5)	4124(3)	2304(7)	2892(3)	113(3)
C(11)	5145(4)	3872(5)	1309(3)	114(2)
C(12)	4098(4)	4167(6)	1902(4)	123(3)
C(13)	3890(5)	4483(8)	2475(6)	160(4)
C(14)	3909(6)	4792(12)	1375(6)	235(8)
C(15)	5521(3)	4494(4)	2661(4)	101(2)
C(16)	5347(5)	4752(6)	3298(5)	139(3)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 35

C(17)		5657(8)	5360(7)	2344(7)	209(6)
C(21)		6584(3)	2779(4)	2266(3)	87(2)
C(22)		6619(3)	2215(4)	3577(3)	87(2)
C(23)		6494(4)	3065(6)	3906(3)	116(2)
C(24)		7366(3)	2095(6)	3697(4)	134(3)
C(25)		6405(2)	932(3)	2503(3)	75(1)
C(26)		6412(4)	272(4)	3043(4)	107(2)
C(27)		7015(3)	849(5)	2258(4)	103(2)
C(31)		5330(3)	1632(8)	938(3)	137(3)
C(32)		4589(6)	319(5)	1427(4)	134(4)
C(33)	#	5045(6)	-355(5)	1780(6)	94(3)
C(34)	#	4216(8)	-170(8)	701(7)	125(5)
C(35)		3981(3)	2006(4)	827(3)	85(1)
C(36)		3347(3)	1837(8)	1013(5)	161(4)
C(37)		3910(4)	1794(6)	107(3)	137(3)
C(33A)	#	5046(10)	-7(9)	1008(10)	123(7)
C(34A)	#	4054(8)	47(10)	1495(13)	133(8)
B		2771(2)	2931(2)	4657(2)	42(1)
C(41)		2139(2)	3573(2)	4606(2)	44(1)
C(42)		1503(2)	3318(2)	4252(2)	51(1)
C(43)		957(2)	3803(3)	4261(2)	60(1)
C(44)		1010(2)	4572(3)	4614(2)	64(1)
C(45)		1626(2)	4851(3)	4975(2)	57(1)
C(46)		2178(2)	4356(2)	4971(2)	49(1)
C(47)		302(2)	3480(4)	3864(3)	82(1)
C(48)		1709(2)	5665(3)	5385(2)	81(1)
C(51)		2672(2)	2329(2)	3987(2)	42(1)
C(52)		2875(2)	1455(2)	3992(2)	48(1)
C(53)		2789(2)	967(2)	3412(2)	54(1)
C(54)		2504(2)	1352(2)	2798(2)	54(1)
C(55)		2317(2)	2226(2)	2782(2)	48(1)
C(56)		2402(2)	2704(2)	3363(2)	44(1)
C(57)		3016(3)	21(3)	3448(3)	87(2)
C(58)		2030(2)	2678(3)	2135(2)	68(1)
C(61)		3454(2)	3475(2)	4733(1)	42(1)
C(62)		4065(2)	3077(2)	5022(2)	47(1)
C(63)		4645(2)	3507(2)	5074(2)	53(1)
C(64)		4663(2)	4355(3)	4831(2)	59(1)
C(65)		4076(2)	4756(2)	4529(2)	57(1)
C(66)		3486(2)	4322(2)	4484(2)	51(1)
C(67)		5284(2)	3075(3)	5422(2)	74(1)
C(68)		4064(3)	5670(3)	4271(3)	90(2)
C(71)		2801(2)	2326(2)	5312(2)	44(1)
C(72)		2387(2)	1598(2)	5282(2)	50(1)
C(73)		2367(2)	1112(3)	5836(2)	56(1)
C(74)		2769(2)	1328(3)	6455(2)	64(1)
C(75)		3179(2)	2051(3)	6499(2)	62(1)
C(76)		3192(2)	2541(3)	5949(2)	51(1)
C(77)		1905(3)	346(3)	5761(2)	77(1)
C(78)		3615(2)	2359(4)	7163(2)	90(2)
F(47A)	§	-180(2)	3980(4)	3932(4)	145(2)
F(47B)		178(3)	2697(4)	3996(5)	180(4)
F(47C)		242(3)	3529(7)	3240(2)	171(3)
F(48A)		1228(5)	6230(6)	5127(5)	192(5)
F(48B)		2226(5)	6151(5)	5348(6)	181(5)
F(48C)		1774(8)	5517(5)	5968(3)	214(6)
F(57A)		2613(4)	-469(3)	2966(3)	155(3)
F(57B)		2871(4)	-413(2)	3956(3)	125(2)
F(57C)		3590(5)	-87(4)	3491(10)	309(10)
F(58A)		1937(3)	2177(3)	1612(1)	108(2)
F(58B)		1464(3)	3046(4)	2099(2)	132(2)
F(58C)		2398(3)	3350(4)	2041(2)	148(2)
F(67A)		5248(2)	2239(4)	5489(6)	201(5)
F(67B)		5745(2)	3189(5)	5154(3)	134(2)
F(67C)		5517(5)	3386(9)	6010(3)	258(7)
F(68A)		4642(2)	6016(3)	4337(4)	145(2)
F(68B)		3733(3)	5756(3)	3658(2)	123(2)
F(68C)		3755(3)	6230(2)	4610(3)	119(2)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 36

F(77A)	1953(5)	-98(5)	6297(3)	178(4)
F(77B)	1972(3)	-223(3)	5305(4)	128(2)
F(77C)	1283(2)	590(4)	5520(4)	125(2)
F(78A)	3767(5)	1644(9)	7579(3)	227(6)
F(78B)	4224(2)	2518(5)	7128(2)	101(2)
F(78C)	3392(4)	2924(11)	7435(5)	283(9)
F(47D)	277(12)	2805(13)	3488(10)	79(2)
F(47E)	-37(11)	4004(13)	3425(10)	79(2)
F(47F)	-146(10)	3246(15)	4124(10)	79(2)
F(48D)	2285(5)	5777(9)	5824(5)	79(2)
F(48E)	1325(5)	5781(8)	5779(6)	79(2)
F(48F)	1635(6)	6415(7)	5070(5)	79(2)
F(57D)	3504(5)	-154(9)	3918(5)	79(2)
F(57E)	3212(6)	-136(10)	2936(5)	79(2)
F(57F)	2596(5)	-536(8)	3442(7)	79(2)
F(58D)	1925(14)	3491(14)	2110(16)	79(2)
F(58E)	2395(14)	2552(18)	1769(14)	79(2)
F(58F)	1500(11)	2324(17)	1850(14)	79(2)
F(67D)	5743(8)	3628(11)	5604(9)	79(2)
F(67E)	5237(11)	2688(12)	5941(8)	79(2)
F(67F)	5450(9)	2505(11)	5066(8)	79(2)
F(68D)	3517(14)	6070(20)	4167(17)	79(2)
F(68E)	4478(16)	6140(20)	4690(17)	79(2)
F(68F)	4222(17)	5730(30)	3726(14)	79(2)
F(77D)	1431(10)	292(15)	5276(8)	79(2)
F(77E)	1652(10)	292(15)	6213(10)	79(2)
F(77F)	2151(9)	-386(11)	5772(11)	79(2)
F(78D)	3653(6)	3221(8)	7247(7)	79(2)
F(78E)	3383(8)	2095(8)	7629(8)	79(2)
F(78F)	4195(6)	2102(9)	7291(8)	79(2)

Remarks:

Isopropyl group C(33)-C(32)-C(34) orientation disordered for C(33) and C(34) with two orientations occupied by 57(1) and 43(1)%.

§ All CF_3 groups were refined with split positions for F with each three F sites (A,B,C) of predominant occupation refined with anisotropic temperature factors without restraints and with further each three F sites (D,E,F) of subordinate occupation with a single isotropic temperature factor and with C-F and F-F distance restraints. Refined site occupation factors for the predominately (A,B,C)/subordinately (D,E,F) occupied fluorine sites were F(47#) 0.834(6)/0.166(6), F(48#) 0.728(8)/0.272(8), F(57#) 0.759(6)/0.241(6), F(58#) 0.904(5)/0.096(5), F(67#) 0.835(6)/0.165(6), F(68#) 0.923(6)/0.077(6), F(77#) 0.851(8)/0.149(8), and F(78#) 0.773(8)/0.227(8).

Table S18. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[CpRu(PMe^iPr_2)_3][BAr'_4]$ - **3**.

	x	y	z	U_{eq}
H(1)	4759	3074	3624	120
H(2)	5499	1709	3853	131
H(3)	4882	536	3071	140
H(4)	3863	1140	2346	153
H(5)	3773	2689	2710	136
H(11A)	5109	4499	1202	171
H(11B)	4839	3542	962	171
H(11C)	5587	3672	1346	171
H(12)	3811	3651	1739	148
H(13A)	3450	4719	2324	240
H(13B)	4186	4944	2702	240
H(13C)	3898	3994	2777	240
H(14A)	3463	4981	1327	353
H(14B)	3939	4520	966	353
H(14C)	4198	5302	1475	353
H(15)	5948	4187	2808	121
H(16A)	5669	5168	3549	208

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 37

H(16B)	5344	4226	3563	208
H(16C)	4917	5026	3185	208
H(17A)	5956	5721	2675	313
H(17B)	5250	5679	2167	313
H(17C)	5852	5228	1987	313
H(21A)	7045	2625	2403	131
H(21B)	6531	3392	2380	131
H(21C)	6414	2702	1791	131
H(22)	6478	1730	3824	104
H(23A)	6764	3075	4362	174
H(23B)	6036	3095	3898	174
H(23C)	6602	3569	3670	174
H(24A)	7585	2179	4164	202
H(24B)	7526	2528	3438	202
H(24C)	7455	1503	3564	202
H(25)	6046	726	2123	90
H(26A)	6551	-301	2923	161
H(26B)	5975	221	3099	161
H(26C)	6712	470	3455	161
H(27A)	7093	230	2183	155
H(27B)	7389	1091	2588	155
H(27C)	6949	1175	1846	155
H(31A)	5156	1333	517	206
H(31B)	5739	1356	1177	206
H(31C)	5407	2251	859	206
H(32)	4242	282	1658	161
H(33A)	4810	-902	1793	141
H(33B)	5250	-155	2229	141
H(33C)	5379	-455	1552	141
H(34A)	4012	278	379	187
H(34B)	3886	-578	763	187
H(34C)	4537	-493	542	187
H(35)	4038	2656	858	102
H(36A)	2982	2091	677	241
H(36B)	3374	2109	1438	241
H(36C)	3281	1204	1041	241
H(37A)	3510	2058	-167	206
H(37B)	3893	1157	45	206
H(37C)	4282	2033	-20	206
H(32A)	4873	174	1874	161
H(33D)	5309	484	928	184
H(33E)	4783	-238	587	184
H(33F)	5331	-471	1247	184
H(34D)	3773	549	1509	200
H(34E)	4131	-286	1905	200
H(34F)	3843	-332	1124	200
H(42)	1449	2795	3998	61
H(44)	636	4906	4612	77
H(46)	2591	4556	5222	59
H(52)	3078	1184	4400	58
H(54)	2441	1024	2405	64
H(56)	2274	3302	3336	53
H(62)	4076	2495	5185	57
H(64)	5062	4648	4872	71
H(66)	3092	4615	4277	61
H(72)	2111	1431	4868	60
H(74)	2764	995	6832	77
H(76)	3471	3034	6002	61

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S19. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[CpRu(PMe^iPr_2)_3][BAr'_4]$ - **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 38

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	45(1)	97(1)	54(1)	18(1)	17(1)	-4(1)
P(1)	63(1)	106(1)	83(1)	40(1)	29(1)	23(1)
P(2)	43(1)	76(1)	59(1)	14(1)	10(1)	-3(1)
P(3)	58(1)	109(1)	56(1)	16(1)	11(1)	8(1)
C(1)	114(5)	125(5)	83(4)	0(3)	63(4)	-23(4)
C(2)	101(4)	168(7)	66(3)	36(4)	37(3)	-26(5)
C(3)	145(7)	111(5)	130(6)	36(4)	100(6)	-5(5)
C(4)	106(5)	188(9)	106(5)	-7(6)	61(5)	-53(6)
C(5)	64(3)	207(9)	80(4)	25(5)	39(3)	2(4)
C(11)	106(4)	146(6)	100(4)	61(4)	48(4)	17(4)
C(12)	111(5)	152(7)	115(5)	39(5)	45(4)	63(5)
C(13)	117(6)	167(8)	193(10)	-9(8)	36(6)	36(6)
C(14)	178(10)	360(20)	165(10)	105(12)	38(8)	170(13)
C(15)	97(4)	90(4)	125(5)	26(3)	48(4)	5(3)
C(16)	140(7)	139(7)	152(8)	4(6)	63(6)	-1(5)
C(17)	350(20)	103(6)	204(12)	23(7)	128(13)	-34(9)
C(21)	61(3)	97(4)	111(4)	28(3)	36(3)	-2(2)
C(22)	62(3)	106(4)	79(3)	-7(3)	-2(2)	-1(2)
C(23)	108(5)	147(6)	87(4)	-26(4)	15(3)	-28(4)
C(24)	68(3)	180(8)	126(6)	-39(5)	-22(4)	8(4)
C(25)	63(2)	80(3)	83(3)	0(2)	19(2)	-2(2)
C(26)	129(5)	84(4)	113(5)	21(3)	39(4)	7(3)
C(27)	70(3)	113(5)	133(5)	-8(4)	38(3)	9(3)
C(31)	90(4)	272(11)	54(3)	25(4)	26(3)	28(5)
C(32)	204(10)	113(5)	102(5)	27(4)	67(6)	75(6)
C(33)	107(7)	51(4)	123(8)	14(5)	28(6)	-11(4)
C(34)	159(12)	79(6)	109(9)	-13(6)	-8(8)	-26(7)
C(35)	68(3)	84(3)	82(3)	5(2)	-16(2)	1(2)
C(36)	57(3)	227(11)	169(8)	36(8)	-18(4)	1(5)
C(37)	144(7)	149(6)	81(4)	-6(4)	-33(4)	15(5)
C(32A)	204(10)	113(5)	102(5)	27(4)	67(6)	75(6)
C(33A)	155(16)	64(7)	154(16)	-25(9)	50(13)	-18(9)
C(34A)	85(10)	77(8)	250(30)	13(11)	63(13)	-18(7)
B	43(2)	45(2)	34(1)	1(1)	6(1)	1(1)
C(41)	46(2)	45(2)	38(1)	-1(1)	8(1)	2(1)
C(42)	47(2)	58(2)	46(2)	4(1)	10(1)	-2(1)
C(43)	45(2)	78(2)	58(2)	14(2)	16(2)	3(2)
C(44)	54(2)	77(3)	67(2)	14(2)	26(2)	24(2)
C(45)	68(2)	57(2)	48(2)	2(2)	19(2)	17(2)
C(46)	51(2)	52(2)	41(2)	-4(1)	6(1)	8(1)
C(47)	49(2)	103(4)	90(3)	15(3)	15(2)	-2(2)
C(48)	93(3)	81(3)	68(3)	-14(2)	22(2)	28(3)
C(51)	44(2)	43(2)	36(1)	-1(1)	8(1)	-2(1)
C(52)	56(2)	43(2)	45(2)	0(1)	15(1)	0(1)
C(53)	71(2)	44(2)	52(2)	-5(1)	24(2)	0(2)
C(54)	62(2)	55(2)	44(2)	-11(1)	16(1)	-9(2)
C(55)	46(2)	57(2)	37(1)	-1(1)	6(1)	-5(1)
C(56)	46(2)	45(2)	40(1)	3(1)	9(1)	4(1)
C(57)	133(5)	57(2)	79(3)	-10(2)	43(3)	-1(3)
C(58)	73(3)	84(3)	39(2)	0(2)	2(2)	5(2)
C(61)	47(2)	43(2)	35(1)	-1(1)	8(1)	1(1)
C(62)	50(2)	49(2)	44(2)	3(1)	12(1)	8(1)
C(63)	45(2)	65(2)	50(2)	3(2)	14(1)	8(2)
C(64)	49(2)	61(2)	65(2)	-1(2)	14(2)	-4(2)
C(65)	55(2)	49(2)	66(2)	5(2)	19(2)	0(2)
C(66)	52(2)	44(2)	53(2)	4(1)	11(1)	6(1)
C(67)	52(2)	88(3)	79(3)	10(2)	14(2)	16(2)
C(68)	84(3)	58(3)	132(5)	24(3)	39(3)	-7(2)
C(71)	44(2)	49(2)	38(1)	-2(1)	10(1)	6(1)
C(72)	52(2)	58(2)	42(2)	0(1)	13(1)	2(2)
C(73)	56(2)	61(2)	53(2)	10(2)	22(2)	4(2)
C(74)	61(2)	87(3)	47(2)	23(2)	21(2)	12(2)
C(75)	51(2)	94(3)	38(2)	9(2)	10(1)	4(2)
C(76)	49(2)	65(2)	38(2)	-2(1)	10(1)	1(2)
C(77)	90(3)	72(3)	78(3)	14(2)	39(3)	-5(2)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 39

C(78)	70(3)	153(5)	42(2)	16(3)	6(2)	-8(3)
F(47A)	43(2)	166(5)	209(6)	-21(4)	7(2)	20(2)
F(47B)	76(3)	105(3)	310(10)	67(5)	-30(4)	-40(3)
F(47C)	91(3)	321(10)	85(3)	-25(4)	-3(2)	-89(5)
F(48A)	163(7)	142(5)	216(8)	-95(6)	-38(6)	103(5)
F(48B)	185(7)	92(4)	306(13)	-111(6)	137(8)	-50(4)
F(48C)	470(20)	113(5)	56(3)	-36(3)	70(6)	-25(7)
F(57A)	289(10)	57(2)	93(4)	-28(2)	12(4)	4(3)
F(57B)	238(7)	43(2)	100(4)	10(2)	55(4)	13(3)
F(57C)	177(7)	72(3)	770(30)	100(8)	292(13)	67(4)
F(58A)	153(4)	123(3)	34(1)	-11(1)	4(2)	27(3)
F(58B)	130(4)	196(5)	62(2)	25(3)	13(2)	93(4)
F(58C)	173(5)	156(4)	84(3)	70(3)	-17(3)	-58(4)
F(67A)	60(2)	117(4)	415(14)	136(7)	47(5)	42(3)
F(67B)	57(2)	167(5)	190(6)	63(4)	55(3)	38(3)
F(67C)	194(7)	411(15)	106(4)	-77(6)	-65(5)	219(10)
F(68A)	89(3)	75(2)	277(7)	57(3)	59(4)	-13(2)
F(68B)	146(4)	99(3)	114(3)	62(2)	17(3)	-7(3)
F(68C)	153(4)	55(2)	155(4)	0(2)	55(3)	12(2)
F(77A)	216(7)	174(6)	111(4)	84(4)	-9(4)	-112(5)
F(77B)	172(5)	86(3)	161(6)	-41(3)	103(5)	-52(3)
F(77C)	70(2)	106(3)	206(6)	6(4)	50(3)	-18(2)
F(78A)	161(7)	369(13)	92(4)	132(6)	-61(4)	-109(9)
F(78B)	77(2)	152(4)	59(2)	15(2)	-8(2)	-29(3)
F(78C)	115(5)	560(20)	144(6)	-239(11)	-18(4)	77(9)

Table S20. Bond lengths [Å] and angles [deg] for $[CpRu(PMe^{i}Pr_2)_3][BAr'_4]$ - **3**. Note that isopropyl group C(33)-C(32)-C(34) is orientation disordered and that CF_3 groups were refined in two orientations with F(#A,B,C) sites predominantely occupied.

Bond distances

Ru-C(3)	2.222(5)
Ru-C(5)	2.240(5)
Ru-C(2)	2.241(5)
Ru-C(1)	2.245(5)
Ru-C(4)	2.246(6)
Ru-P(2)	2.3555(14)
Ru-P(3)	2.3657(17)
Ru-P(1)	2.3678(17)
P(1)-C(11)	1.859(6)
P(1)-C(15)	1.872(8)
P(1)-C(12)	1.889(7)
P(2)-C(21)	1.813(5)
P(2)-C(25)	1.876(5)
P(2)-C(22)	1.880(6)
P(3)-C(31)	1.860(6)
P(3)-C(35)	1.881(5)
P(3)-C(32)	1.882(9)
C(1)-C(5)	1.397(10)
C(1)-C(2)	1.420(11)
C(1)-H(1)	0.94
C(2)-C(3)	1.419(11)
C(2)-H(2)	0.94
C(3)-C(4)	1.361(12)
C(3)-H(3)	0.94
C(4)-C(5)	1.379(12)
C(4)-H(4)	0.94
C(5)-H(5)	0.94
C(11)-H(11A)	0.97
C(11)-H(11B)	0.97
C(11)-H(11C)	0.97
C(12)-C(14)	1.424(13)
C(12)-C(13)	1.471(13)
C(12)-H(12)	0.99
C(13)-H(13A)	0.97
C(13)-H(13B)	0.97
C(13)-H(13C)	0.97
C(14)-H(14A)	0.97
C(14)-H(14B)	0.97
C(14)-H(14C)	0.97
C(15)-C(17)	1.530(11)
C(15)-C(16)	1.533(11)
C(15)-H(15)	0.99
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
C(16)-H(16C)	0.97
C(17)-H(17A)	0.97
C(17)-H(17B)	0.97
C(17)-H(17C)	0.97
C(21)-H(21A)	0.97
C(21)-H(21B)	0.97
C(21)-H(21C)	0.97
C(22)-C(23)	1.514(10)
C(22)-C(24)	1.550(9)
C(22)-H(22)	0.99
C(23)-H(23A)	0.97
C(23)-H(23B)	0.97
C(23)-H(23C)	0.97
C(24)-H(24A)	0.97
C(24)-H(24B)	0.97
C(24)-H(24C)	0.97
C(25)-C(26)	1.506(8)

© 2001 American Chemical Society, Organometallics, Aneetha om010730v Supporting Info Page 40

C(25)-C(27)	1.526(7)
C(25)-H(25)	0.99
C(26)-H(26A)	0.97
C(26)-H(26B)	0.97
C(26)-H(26C)	0.97
C(27)-H(27A)	0.97
C(27)-H(27B)	0.97
C(27)-H(27C)	0.97
C(31)-H(31A)	0.97
C(31)-H(31B)	0.97
C(31)-H(31C)	0.97
C(32)-C(33)	1.459(12)
C(32)-C(34)	1.682(15)
C(32)-H(32)	0.99
C(33)-H(33A)	0.97
C(33)-H(33B)	0.97
C(33)-H(33C)	0.97
C(34)-H(34A)	0.97
C(34)-H(34B)	0.97
C(34)-H(34C)	0.97
C(35)-C(37)	1.511(10)
C(35)-C(36)	1.525(11)
C(35)-H(35)	0.99
C(36)-H(36A)	0.97
C(36)-H(36B)	0.97
C(36)-H(36C)	0.97
C(37)-H(37A)	0.97
C(37)-H(37B)	0.97
C(37)-H(37C)	0.97
C(33A)-H(33D)	0.97
C(33A)-H(33E)	0.97
C(33A)-H(33F)	0.97
C(34A)-H(34D)	0.97
C(34A)-H(34E)	0.97
C(34A)-H(34F)	0.97
B-C(71)	1.635(5)
B-C(41)	1.636(5)
B-C(61)	1.637(5)
B-C(51)	1.638(4)
C(41)-C(46)	1.398(5)
C(41)-C(42)	1.404(5)
C(42)-C(43)	1.378(5)
C(42)-H(42)	0.94
C(43)-C(44)	1.366(6)
C(43)-C(47)	1.493(6)
C(44)-C(45)	1.385(6)
C(44)-H(44)	0.94
C(45)-C(46)	1.394(5)
C(45)-C(48)	1.483(6)
C(46)-H(46)	0.94
C(47)-F(47B)	1.259(7)
C(47)-F(47F)	1.273(15)
C(47)-F(47E)	1.274(15)
C(47)-F(47D)	1.281(15)
C(47)-F(47C)	1.283(7)
C(47)-F(47A)	1.312(7)
C(48)-F(48C)	1.214(8)
C(48)-F(48F)	1.299(10)
C(48)-F(48D)	1.323(10)
C(48)-F(48E)	1.326(9)
C(48)-F(48A)	1.327(7)
C(48)-F(48B)	1.340(8)
C(51)-C(52)	1.388(4)
C(51)-C(56)	1.397(4)
C(52)-C(53)	1.390(5)
C(52)-H(52)	0.94
C(53)-C(54)	1.392(5)
C(53)-C(57)	1.502(6)
C(54)-C(55)	1.376(5)
C(54)-H(54)	0.94
C(55)-C(56)	1.384(5)
C(55)-C(58)	1.491(5)
C(56)-H(56)	0.94
C(57)-F(57C)	1.210(9)
C(57)-F(57F)	1.225(9)
C(57)-F(57D)	1.246(10)
C(57)-F(57E)	1.278(10)
C(57)-F(57A)	1.352(7)
C(57)-F(57B)	1.359(7)
C(58)-F(58F)	1.24(2)
C(58)-F(58D)	1.25(2)
C(58)-F(58E)	1.25(2)
C(58)-F(58A)	1.302(5)
C(58)-F(58B)	1.309(6)
C(58)-F(58C)	1.329(6)
C(61)-C(66)	1.390(5)
C(61)-C(62)	1.407(5)
C(62)-C(63)	1.371(5)
C(62)-H(62)	0.94
C(63)-C(64)	1.383(5)
C(63)-C(67)	1.502(5)
C(64)-C(65)	1.373(5)
C(64)-H(64)	0.94
C(65)-C(66)	1.397(5)
C(65)-C(68)	1.479(6)
C(66)-H(66)	0.94
C(67)-F(67F)	1.254(13)
C(67)-F(67D)	1.260(13)
C(67)-F(67E)	1.263(13)
C(67)-F(67B)	1.271(6)
C(67)-F(67A)	1.274(7)
C(67)-F(67C)	1.284(8)
C(68)-F(68E)	1.28(3)
C(68)-F(68D)	1.28(2)
C(68)-F(68F)	1.28(2)
C(68)-F(68B)	1.292(7)
C(68)-F(68A)	1.306(6)
C(68)-F(68C)	1.383(7)
C(71)-C(72)	1.399(5)
C(71)-C(76)	1.403(4)
C(72)-C(73)	1.386(5)
C(72)-H(72)	0.94
C(73)-C(74)	1.382(6)
C(73)-C(77)	1.497(6)
C(74)-C(75)	1.385(6)
C(74)-H(74)	0.94
C(75)-C(76)	1.377(5)
C(75)-C(78)	1.519(6)
C(76)-H(76)	0.94
C(77)-F(77E)	1.216(15)
C(77)-F(77F)	1.219(15)
C(77)-F(77D)	1.221(15)
C(77)-F(77A)	1.289(6)
C(77)-F(77B)	1.321(7)
C(77)-F(77C)	1.331(7)
C(78)-F(78C)	1.195(10)
C(78)-F(78F)	1.249(11)
C(78)-F(78E)	1.277(11)
C(78)-F(78D)	1.312(11)
C(78)-F(78B)	1.339(7)
C(78)-F(78A)	1.370(10)

Bond angles